Overview of DAKOTA Project
(from the software perspective)

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- Capability overview
- Advanced deployment efforts

Sandia is a multi program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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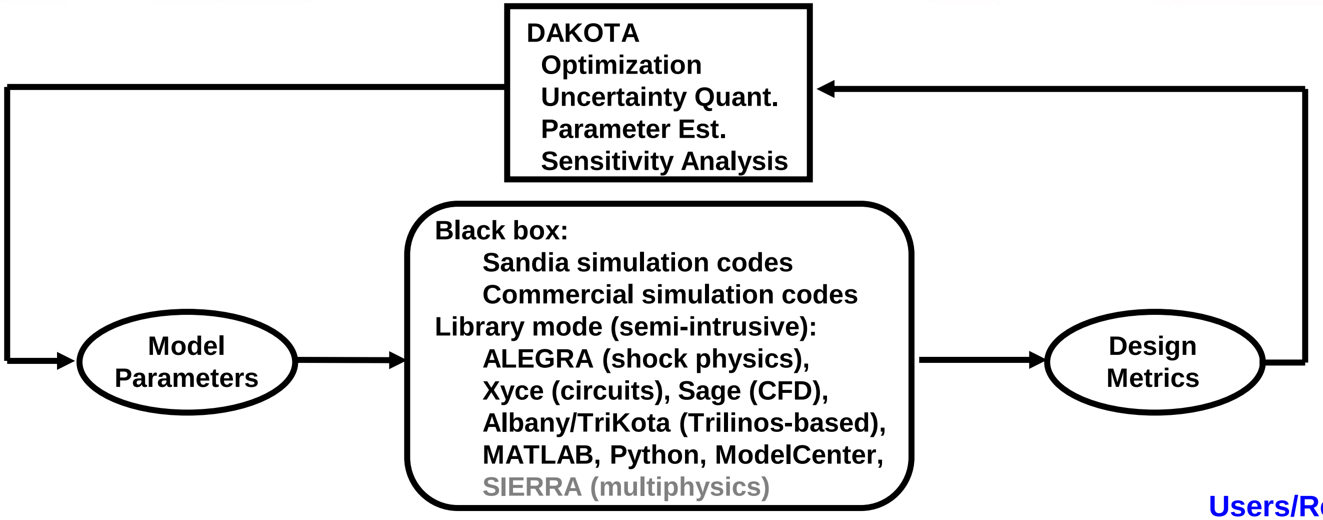
DAKOTA Project



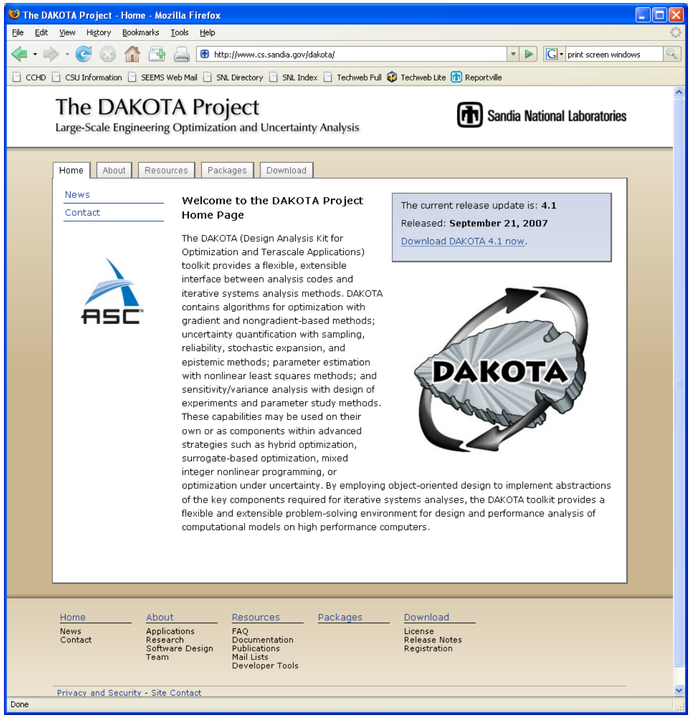
Iterative systems analysis

Multilevel parallel computing

Simulation management

http://dakota.sandia.gov

Users/Ref/Dev Manuals + training matls. online



Began as optimization LDRD in 1994

Team: 5-10 core personnel in NM/CA + TPL developers

Releases: Major/Interim, Stable/VOTD; *5.1 release due 12/10*

DAKOTA Training: 8 sessions (~140 students) since 5.0;
26 sessions (~500 students) total since 2001.

2009 Outreach: Minitutorials at IMAC, SIAM CS&E;
SA/UQ short courses at NASA Langley, AFRL WPAFB.

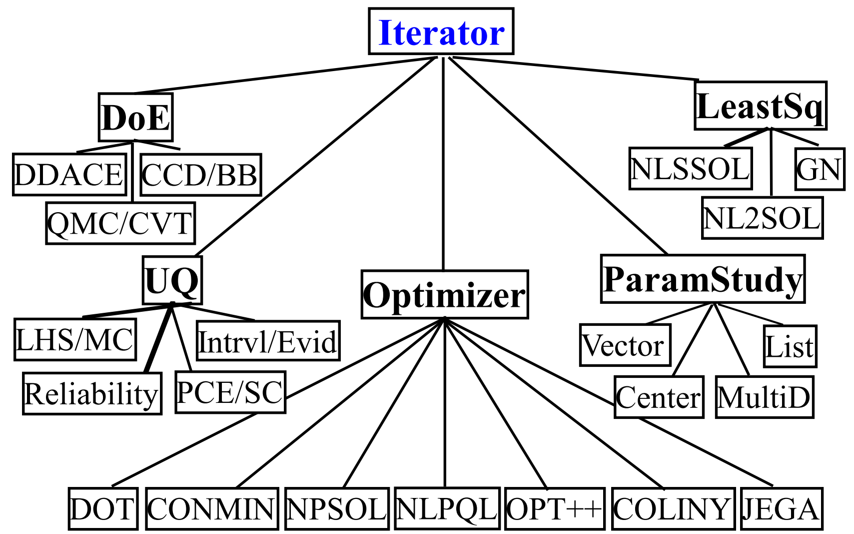
Modern SQE: Linux/Unix, Mac, Windows; Nightly builds/testing;
subversion, TRAC, Cmake; Top 2008 SQE score

GNU LGPL: free downloads worldwide
(~6500 total ext. registrations, ~3500 distributions last yr.)

Community development: open checkouts now avail (→ PSAAP)

Community support: dakota-users, dakota-developers

C++ Framework



Model:

Design
- continuous
- discrete range/set

Uncertain
- normal/lognorm.
- uniform/logunif.
- triang/exp/β/Γ
- EV: I, II, III
- histogram: bin/pt
- discrete: p/b/nb/g/hg
- interval

State
- continuous
- discrete range/set

Application
- system
- fork
- direct
- grid

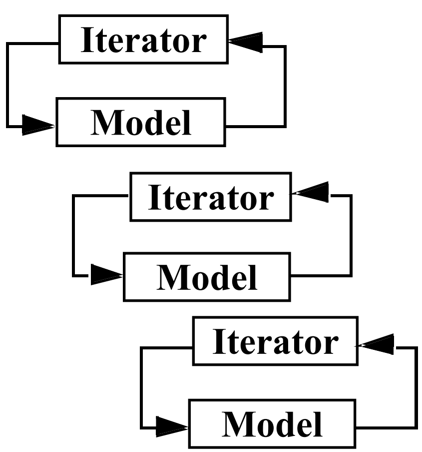
Approximation
- global
  - polynomial 1/2/3, NN, kriging, MARS, RBF
- multipoint – TANA3
- local – Taylor series
- multifidelity
- ROM

Functions
- objectives
- nonlin constraints
- least sq. terms
- generic

Gradients
- numerical
- analytic

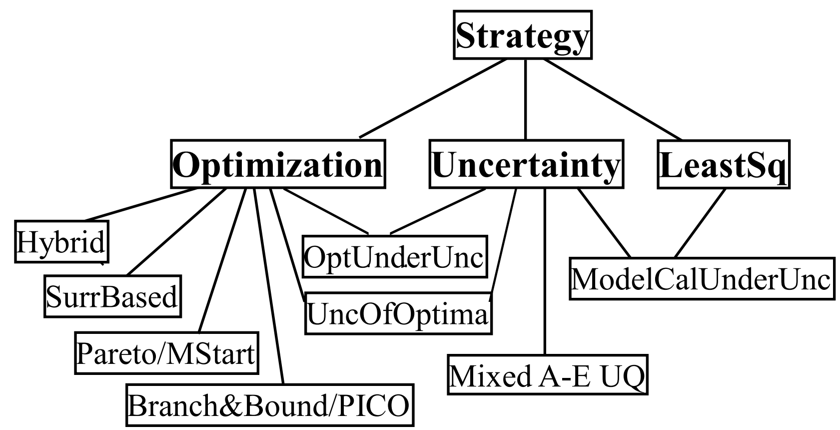
Hessians
- numerical
- analytic
- quasi

Strategy: control of multiple iterators and models



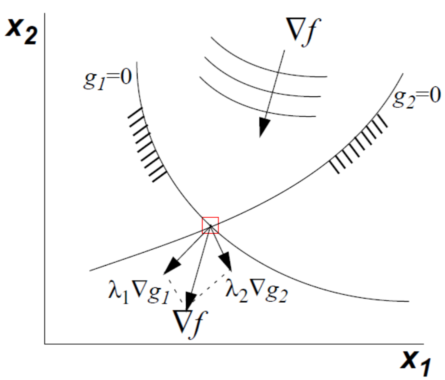
Coordination:
- Nested
- Surrogate
- Recast
- Sequential/Concurrent
- Adaptive/Interactive

Parallelism:
- Asynchronous local
- Message passing
- Hybrid
- 4 nested levels with
  - Master-slave/dynamic
  - Peer/static



Core Methods

Optimization: minimize/maximize objective(s) subject to constraints

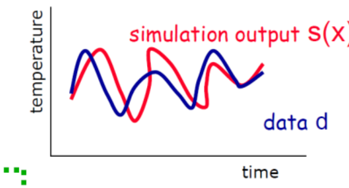


Karush-Kuhn-Tucker conditions:

$$\nabla f - \sum_i \lambda_i \nabla g_i = 0$$

Achieve vector balance: objective fn grad contained within feasibility cone

Model Calibration/Parameter Estimation: use nonlinear least squares to minimize errors between model and data

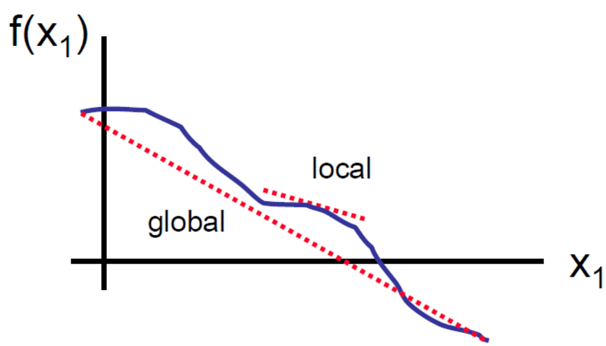


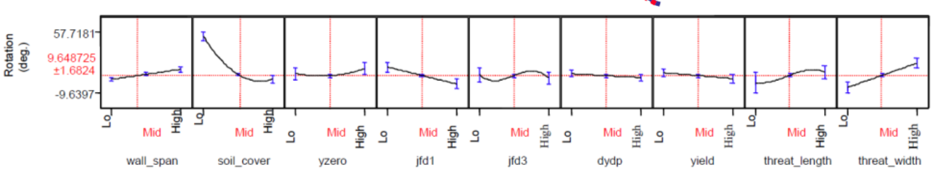
$$f(x) = \sum_{i=1}^{n} (s_i(x) - d_i)^2$$

Simulation output that depends on x

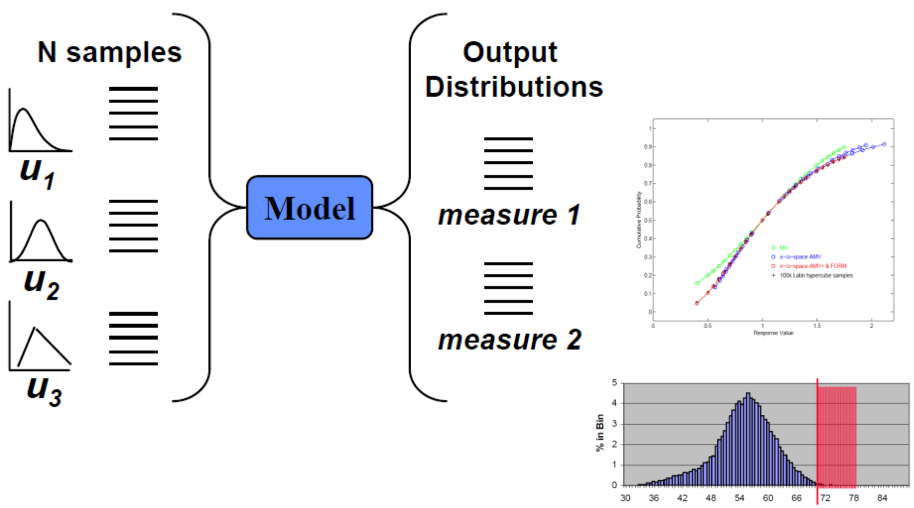
Given data

Sensitivity Analysis: identify most influential set of parameters for key response metrics





Uncertainty Quantification: quantify effect of random variables on key response metrics



Uncertainty Quantification Algorithms @ SNL: New methods bridge robustness/efficiency gap

	Production	New	Under dev.	Planned	Collabs.
Sampling	Latin Hypercube, Monte Carlo	Importance, Incremental		Bootstrap, Jackknife	FSU
Reliability	*Local:* Mean Value, First-order & second-order reliability methods (FORM, SORM)	*Global:* Efficient global reliability analysis (EGRA)		gradient-enhanced EGRA	*Local:* Notre Dame, *Global:* Vanderbilt
Stochastic expansion		Tailored polynomial chaos & stochastic collocation with extended basis selections	p-adaptive, adjoint gradient-enhanced	h-adaptive, hp-adaptive, discrete, multi-physics	Stanford, Purdue, Austr. Natl., FSU
Other probabilistic		Random fields/ stochastic proc.		Dimension reduction	Cornell, Maryland
Epistemic	Interval-valued/ Second-order prob. (nested sampling)	Opt-based interval estimation, Dempster-Shafer	Bayesian	Imprecise probability	LANL, Applied Biometrics
Metrics & Global SA	Importance factors, Partial correlations	Main effects, Variance-based decomposition	Stepwise regression		UNM

Reseach: Tailoring & Adaptivity

Adv. Deployment

Fills Gaps

Generalized Polynomial Chaos Expansions

Approximate response w/ spectral proj. using orthogonal polynomial basis fns

i.e. $$R = \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi})$$ using

$$\begin{aligned}
\Psi_0(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_0(\xi_2) = 1 \\
\Psi_1(\boldsymbol{\xi}) &= \psi_1(\xi_1)\,\psi_0(\xi_2) = \xi_1 \\
\Psi_2(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_1(\xi_2) = \xi_2 \\
\Psi_3(\boldsymbol{\xi}) &= \psi_2(\xi_1)\,\psi_0(\xi_2) = \xi_1^2 - 1 \\
\Psi_4(\boldsymbol{\xi}) &= \psi_1(\xi_1)\,\psi_1(\xi_2) = \xi_1\xi_2 \\
\Psi_5(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_2(\xi_2) = \xi_2^2 - 1
\end{aligned}$$

- Nonintrusive: estimate α_j using sampling (expectation), pt collocation (regression), tensor-product quadrature, Smolyak sparse grids, or cubature (numerical integration)

$$\alpha_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int_\Omega R\, \Psi_j\, \varrho(\boldsymbol{\xi})\, d\boldsymbol{\xi}$$

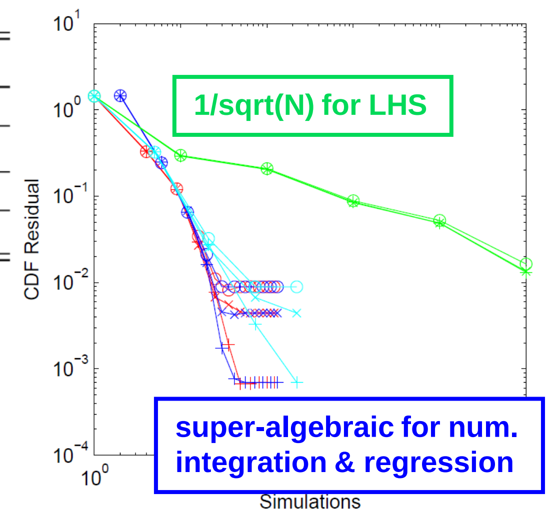
$$\langle \Psi_j^2 \rangle = \prod_{i=1}^{n} \langle \psi_{m_i^j}^2 \rangle$$

Generalized PCE (Wiener-Askey + numerically-generated)

- Tailor basis: optimal basis selection leads to exponential convergence rates

Distribution	Density function	Polynomial	Weight function	Support range
Normal	$\frac{1}{\sqrt{2\pi}} e^{\frac{-x^2}{2}}$	Hermite $He_n(x)$	$e^{\frac{-x^2}{2}}$	$[-\infty, \infty]$
Uniform	$\frac{1}{2}$	Legendre $P_n(x)$	1	$[-1, 1]$
Beta	$\frac{(1-x)^\alpha (1+x)^\beta}{2^{\alpha+\beta+1} B(\alpha+1,\beta+1)}$	Jacobi $P_n^{(\alpha,\beta)}(x)$	$(1-x)^\alpha (1+x)^\beta$	$[-1, 1]$
Exponential	e^{-x}	Laguerre $L_n(x)$	e^{-x}	$[0, \infty]$
Gamma	$\frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)}$	Generalized Laguerre $L_n^{(\alpha)}(x)$	$x^\alpha e^{-x}$	$[0, \infty]$

Additional bases generated numerically via Golub-Welsch



- Tailor expansion type/order/range:
  - Total order → tensor and sum of tensor expansions
  - Dimension p-refinement: anisotropic tensor/sparse grids
  - Domain h-refinement: discretization of random domain

ASCR Wind Turbine UQ

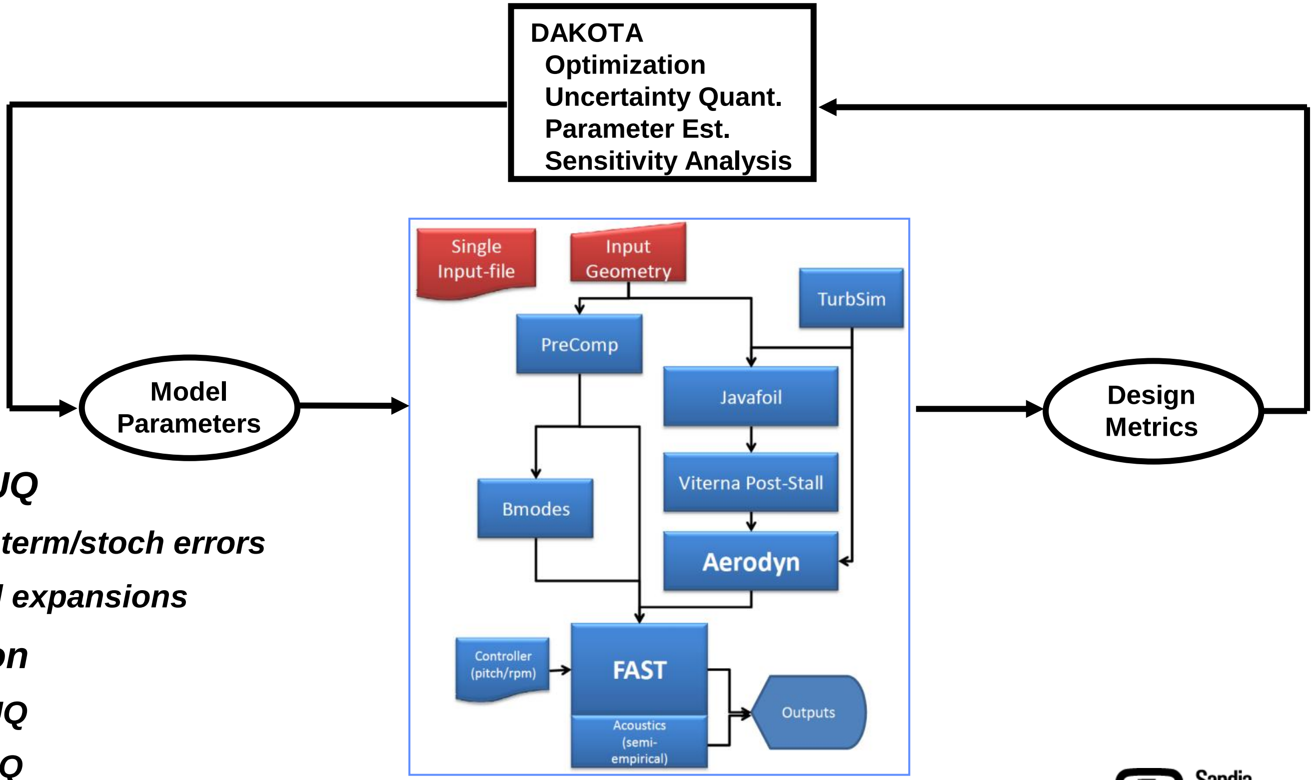
New DOE ASCR Project (Office of Science): FY2010-2012

Short term:

- ***MATLAB management of NREL design tool ensemble ("EOLO", Sandia wind group)***

Longer term:

- ***CFD with Joe (Stanford) and FSI with SIERRA/Aria (Sandia)***



UQ Research goals

- ***Inner core: probabilistic UQ***
  - ***Adjoint EE → balance of determ/stoch errors***
  - ***Adaptive, adjoint-enhanced expansions***
- ***Aggregation & Data Fusion***
  - ***Mixed Aleatory/Epistemic UQ***
  - ***Model Form: multifidelity UQ***
  - ***Data fusion: Bayesian inference → BMA***

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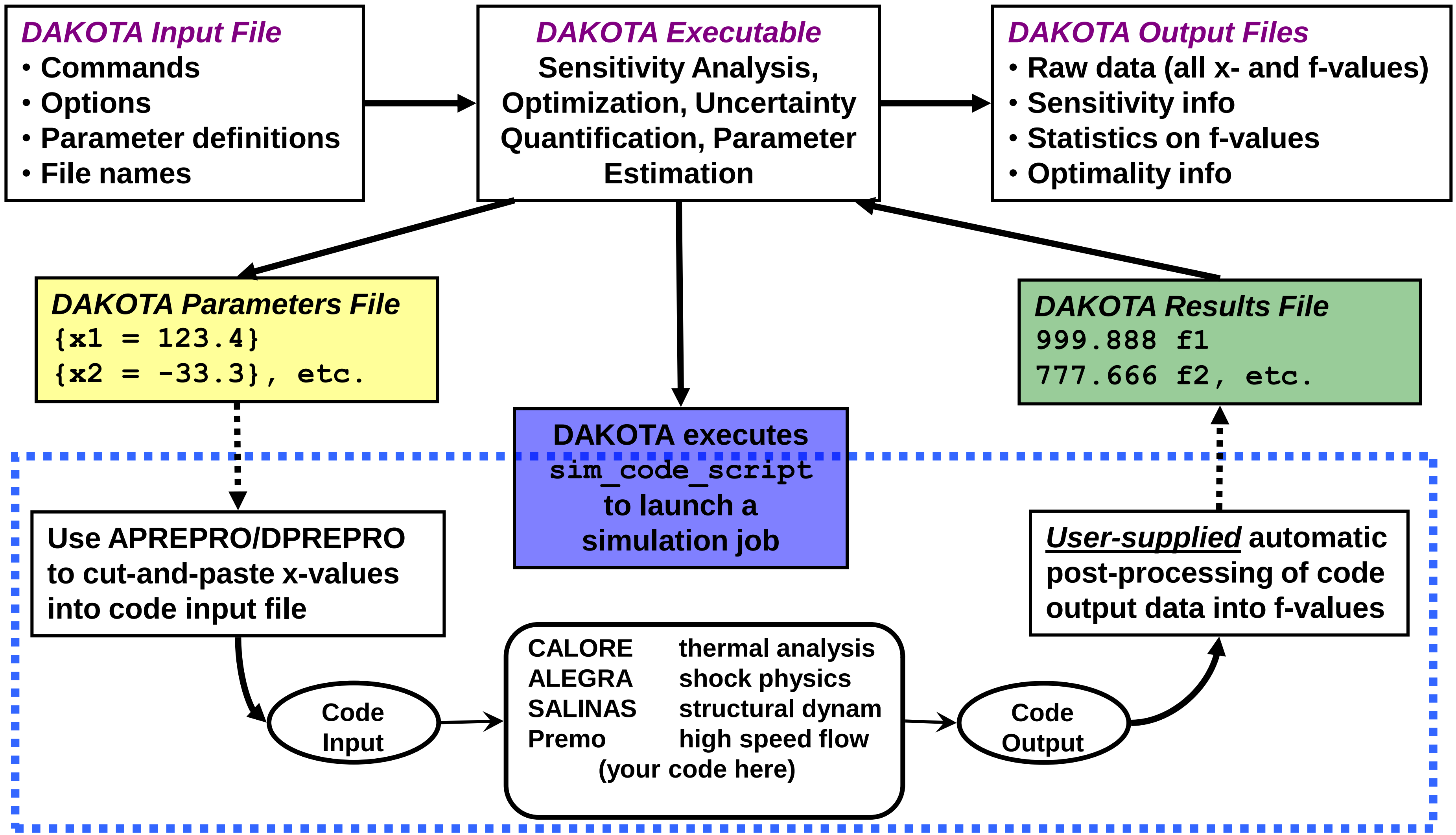
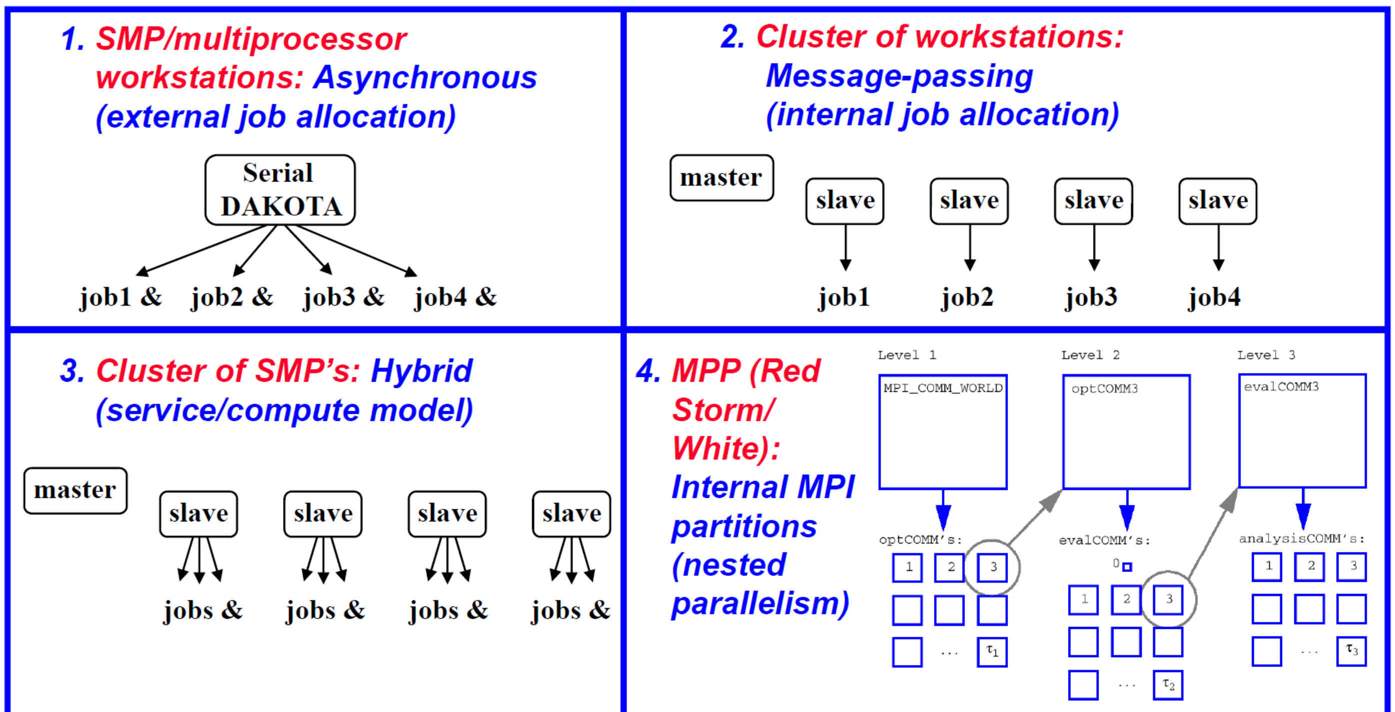
Simulation Management (Black Box case)



Parallelism Options: Multicore Desktops to MPP

1. ***Algorithmic coarse-grained***: **concurrency in data requests:**
   - **Iterators: Gradient-based, Nongradient-based, Surrogate-based**
   - **Strategies with concurrent Iterators: Multi-start, Pareto, Hybrid**
   - **Nested Models: OUU/MCUU, Mixed UQ**
2. ***Algorithmic fine-grained:*** **computing the internal linear algebra of an opt. algorithm in parallel**
3. ***Fn eval coarse-grained:*** **concurrent execution of separable simulations within each fn. eval.**
4. ***Fn eval fine-grained:*** **parallelization of the solution steps within a single analysis code**



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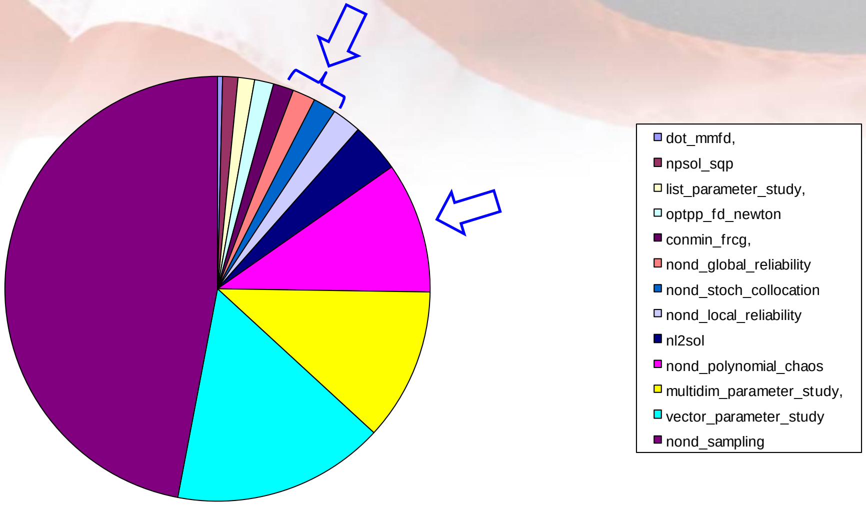
Deployment



Jan/Feb 2010: 92% of DAKOTA invocations on SNL clusters were UQ or param studies, but new methods starting to reduce LHS dominance

Impact Sandia missions

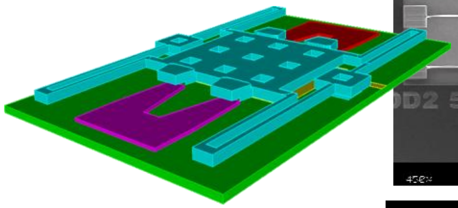
- Technology insertion
  - ASC milestones
  - Early adopters

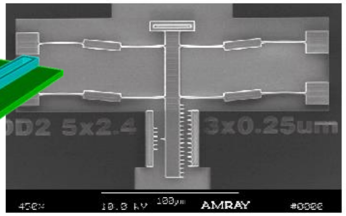
Partnerships

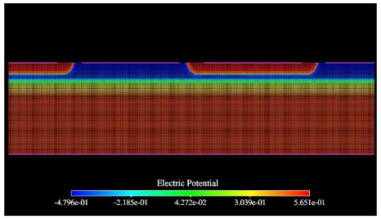
- Government: LLNL, LANL, ORNL, INL, NASA, DOD
- Industry: Lockheed Martin, Goodyear, Exxon Mobil
- University: MIT, Cornell, CU Boulder, Vanderbilt, USC, FSU, Notre Dame, VPISU, UNM
  - CSRI students/postdocs, faculty sabbaticals
  - ASC PSAAP: UT Austin (Bayesian), Purdue (cubature), UIUC (adaptive collocation), Caltech (global opt.), Michigan (gradient-enhanced interpolation), Stanford (adaptive collocation)

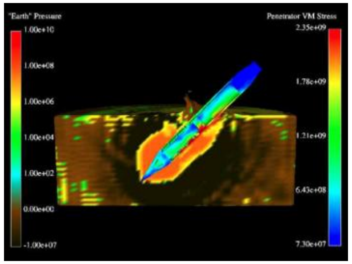
Address core usability barriers

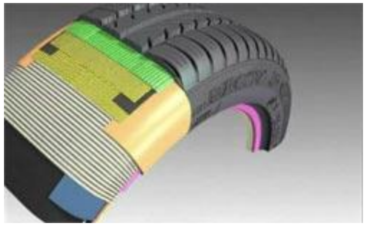
- JAGUAR
- Library embedding

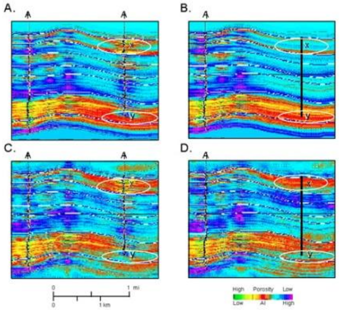


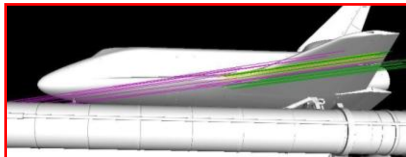










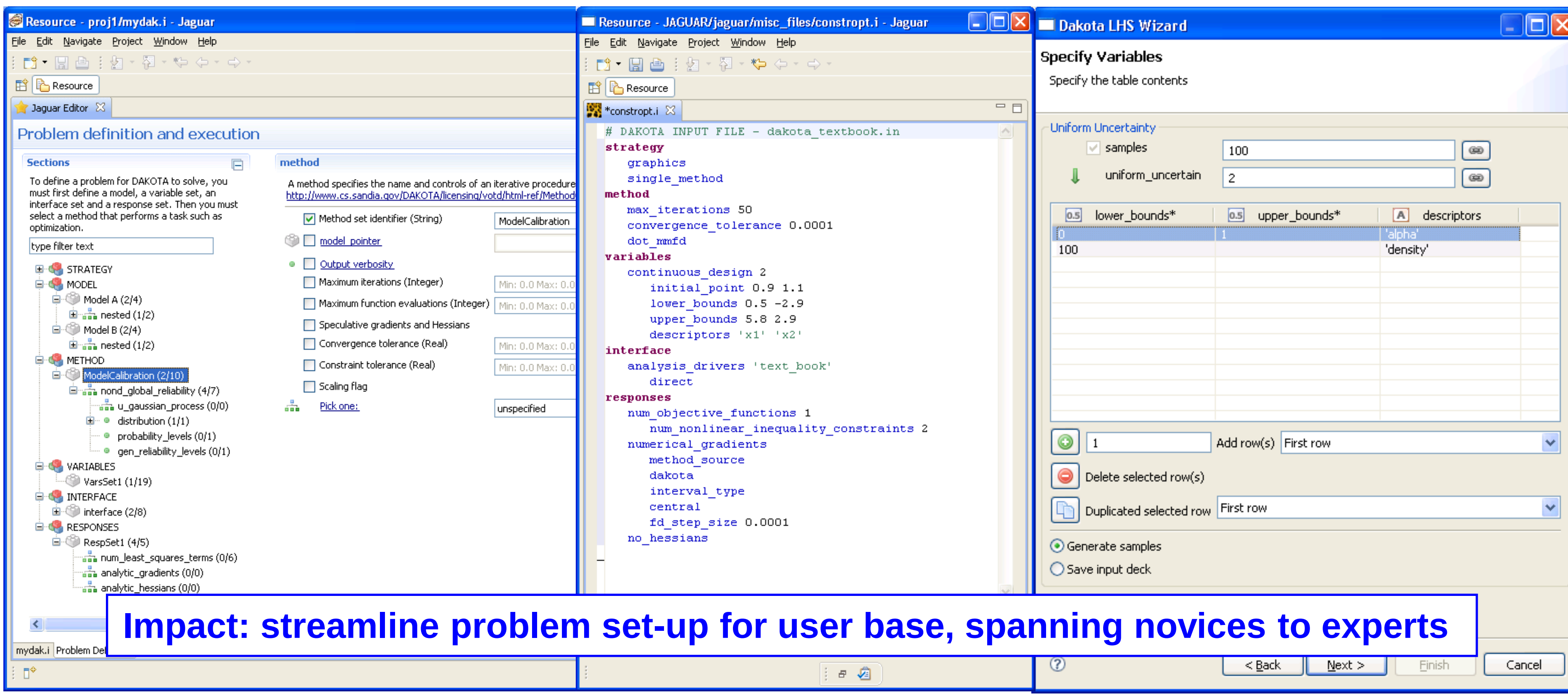


Deployment Initiative: JAGUAR User Interface

- Eclipse-based rendering of full DAKOTA input spec.
- Automatic syntax updates
- Tool tips, Web links, help
- Symbolics, sim. interfacing

- Flat text editor for experienced users
- Keyword completion
- Automatically synchronized with GUI widgets

- Simplified views for high-use applications (“Wizards”)



Impact: streamline problem set-up for user base, spanning novices to experts

Deployment Initiative: Embedding

Make DAKOTA natively available within application codes

- Streamline problem set-up, reduce complexity, and lower barriers
  - A few additional commands within existing simulation input spec.
  - Eliminate analysis driver creation & streamline analysis (e.g., file I/O)
  - Simplify parallel execution
- Integrated options for algorithm intrusion ⇨

ModelEvaluator Levels

Non-intrusive

ModelEvaluator: systems analysis

- All residuals eliminated, coupling satisfied
- DAKOTA optimization & UQ

Intrusive to coupling

ModelEvaluator: multiphysics

- Individual physics residuals eliminated; coupling enforced by opt/UQ
- DAKOTA opt/UQ & MOOCHO opt.

Intrusive to physics

ModelEvaluator: single physics

- MOOCHO opt., Stokhos UQ, NOX, LOCA

SNL Embedding

- Existing: Xyce, Sage, Albany (TriKOTA)
- New: ALEGRA, SIERRA (TriKOTA) → STK

External Embedding

- Existing: ModelCenter, university applications
- New: QUESO (UT Austin), R7 (INL)
- Expanding our external focus:
  - GPL → LGPL; svn restricted → open network

Impact: eliminate custom set-up and support fully integrated opt. and UQ studies

Concluding Remarks

DAKOTA provides a variety of core algorithms for iterative analysis:

– *Optimization* -- *Sensitivity Analysis*

– *Calibration* -- *Uncertainty quantification*

As well as advanced capabilities for

– *Multilevel parallel computing*

– *Manage multiple iterative methods, models of varying fidelity, nesting, recasting, etc.*

– *Emerging UQ methods: adaptive, adjoint-enhanced, multi-{fidelity,physics,scale}, mixed UQ*

– *Emerging algs. in other areas: OUU, SBO, MINLP, SA w/ PCE/SC, Nond. calibration*

Advanced deployment initiatives will "lower the bar" for adoption

– *JAGUAR* -- *Library embedding*

Expanding from NNSA to include energy missions: Wind, NE

Some lessons learned in open source framework development

– *Bound your mission space and manage scope creep*
  - *Focus on your core strengths and provide flexible APIs for others to use*
  - *Be selective on strategic partnerships*

– *Establish a support hierarchy and manage it effectively*
  - *Small teams may need to rely on community support for bottom tier*

– *Utilize modern CS tools (svn/git, cmake/scons, Trac) to simplify collaborative development*

– *Manage quality through sponsorship and review of external contributions*