PECOS V&V/UQ Overview

Center for Predictive Engineering and Computational Science
Institute for Computational Engineering and Sciences
The University of Texas at Austin

DOE PSAAP Kickoff Meeting
Albuquerque, New Mexico
July 9, 2008

Overview of PECOS V&V/UQ Framework

- Verification
  - *Software quality engineering:* Employ professional standards
  - *Code verification:* Employ & advance state-of-the-art methods
  - *Solution verification:* Build on advances in error estimation

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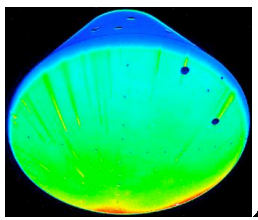
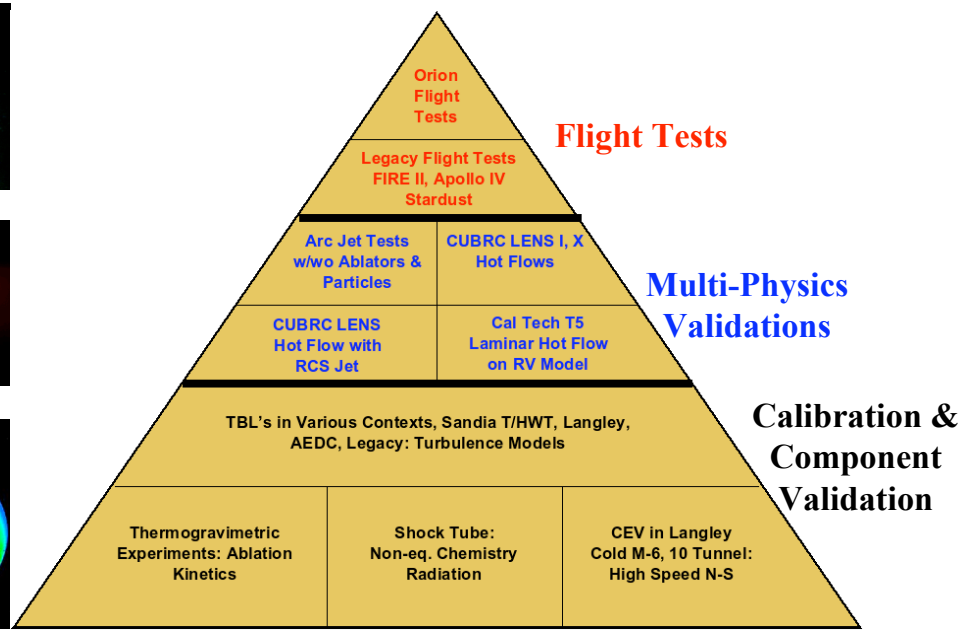
- Prediction
  - *Predict probabilities of quantities of interest* for regimes of interest using validated code

Uncertain Parameters, Experiments, & Validation Pyramid





Uncertain model parameters

- chemical kinetic parameters
- radiation absorption and emission parameters
- ablation kinetic parameters
- turbulence model parameters
- ablative particle density parameters

Tag	Facility	Description	Flow	Measure	Calibrate	Validate	Code	Level
TGM		Thermogavimetric Experiments	N/A	Mass as function of T during slow heating	Ablation kinetics		Ablate	1
ST	EAST	Shock Tube	Hypersonic shock	Radiometry	Chemical, radiation	Aerothermochemistry, radiation emission/absorption	Radiate, Hyflow,	1
NS	Langley	RV model w/wo penetrations	M=6, 10, cold, laminar	q_s, T_s (thermal paint)		High speed Navier-Stokes	Hyflow	1
NSJET	Langley RCS	RV model with RCS jets	M=10, cold, laminar	q_s, P_s Jet Fluid Dilution,		High speed Navier-Stokes	Hyflow	1
TURB1	Sandia HWT	Sphere-cone model	M=5, 8, 14, cold	$P_s, \rho u$, *fluctuating*	Turbulence	Turbulence	Hyflow	1
TURB2	Sandia TWT	Turbulent boundary layer with steady cross-flow jet	M=0.8, cold	$u\,(2-D)$	Turbulence	Turbulence	Hyflow	1
TURB3	Sandia TWT	Turbulent boundary layer	M<3, cold	$P_s, u\,(2-D)$	Turbulence	Turbulence	Hyflow	1
TURB4	Langley	Legacy boundary layer experiments	M<11, cold	$\rho u, T$, *fluctuating*	Turbulence	Turbulence	Hyflow	1
TRAN	AEDC T9	RV model w/wo roughness	M=6, cold	q_s, T_s	Turbulence	Turbulence, transition	Hyflow	1
PART	Arc Jet	Comparison of PICA and copper targets	M<12, hot, long	Part. density by laser extinction, spectroscopy	Particles	Particle generation \& transport	Hyflow	2
ABLATE	Arc Jet	Ablative material flow tests	M<12, hot, long	q_s, T_s, σ_s Recession, rad		All	Hyflow, Ablate, Radiate??	2
HOT1	CUBRC LENS 1	RV model with blowing and/or roughness	M<25, hot	P_s, q_s, T_s, σ_s Schlieren		All except ablation	Hyflow, Radiate	2
HOTJET	CUBRC LENS	RV model with RCS jets	M<25, hot	P_s, q_s, T_s, σ_s Schlieren		All except ablation	Hyflow, Radiate	2
HOT2	CUBRC LENS X	RV model	M<25, hot	P_s, q_s, T_s, σ_s Schlieren, rad.		Turbulence, chemistry, radiation	Hyflow, Radiate	2
HOTLAM	CalTech T5	RV model	M<5,hot laminar	q_s, T_s		Chemistry, radiation, laminar transport	Hyflow, Radiate	2
FLIGHT1	Fire II	Apollo-era flight test		q_s, T_s Radiometry		All	Hyflow, Ablate, Radiate	3
FLIGHT2	Apollo IV	Apollo lunar exchange flight test		q_s, T_s Radiometry		All	Hyflow, Ablate, Radiate	3
FLIGHT3	LEO	CEV Low Earth Orbit flight test		q_s, T_s Radiometry		All	Hyflow, Ablate, Radiate	3
FLIGHT4	LEX	2m capsule lunar exchange flight test		q_s, T_s Radiometry		All	Hyflow, Ablate, Radiate	3
FLIGHT5	Startdust	Comet sample-return mission		TPS Condition		All	Hyflow, Ablate, Radiate	3

Challenges and Opportunities

- Draw on and advance research in manifold areas:
  - Error estimation, adaptivity
  - Inverse problems, estimation of uncertainty
  - Bayesian statistical inference
  - Stochastic PDEs, propagation of uncertainty
  - Large-scale parallel algorithms and computing

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- Mathematical and computational challenges:
  - Methods for verification of multiphysics, multiscale codes
  - Estimation of model uncertainty
  - Scalable methods for statistical inverse problems in high dimensions and for expensive simulations
  - Scalable methods for propagating uncertainty from inputs to outputs in high dimensions and for expensive simulations
  - UQ-aware reduced models
  - Exploitation of upcoming sustained multi-petaflops systems

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- PSAAP provides an outstanding opportunity to:
  - develop rigorous methodology for end-to-end V&V/UQ
  - apply framework to problem of NNSA and national interest