XPACC: The Center for Exascale Simulation of Plasma-Coupled Combustion

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A new DOE/NNSA-funded ASC PSAAP MSC Center
DOE/NNSA/ASC/PSAAP Motivation

► NNSA — DOE National Nuclear Security Administration

► ASC — Office of Advanced Simulation and Computing
  “Established in 1995, the ASC Program supports the U.S. Defense Programs’ shift in emphasis from test-based confidence to simulation-based confidence”

► PSAAP — Predictive Science Academic Alliance Program
  • Multidisciplinary Simulation Centers (MSC) (3 $3.2M/year)
  • Single-discipline Centers (SDC) (3 $1.6M/year)

“We expect the PSAAP alliances will continue to help develop the predictive science field and the workforce of the future, wherein simulations will be pervasive and instrumental in important, high-impact decision-making processes” [emphasis added]

— Robert Meisner, director of NNSA ASC
XPACC MSC Specific Motivation

- Truly predictive simulations will accelerate fundamental advances in the use of plasmas to improve combustion
- Computer Science advances that enable such massive-scale predictive simulations will have broad impact
Specific Target Application

- Predict the ignition threshold of a jet in crossflow via spark-discharge and dielectric-barrier-discharge plasmas
- Iconical combustion flow with new ‘knobs’ for mediating ignition
Coupled-Physics Predictive Science Challenge

- Plasmas introduce chemical-reaction-coupling radicals
- Plasma heating triggers chemistry
- Local heating alter flow/turbulence
- Electric fields alter diffusion of charged species
- Electric fields exert body forces, destabilizing flames
- Electrodes age and alter plasma generation efficacy
- Turbulence mixes reactants
- Flows alters plasma structure
- ...
A Multi-Scale Predictive Science Challenge

▶ LENGTH:
- **nm-scale**
  - electrode surface physics
  - mean-free-path reactions
- **µm-scale**
  - plasma structures
  - flame thickness
- **mm-scale**
  - turbulence
- **m-scale**
  - device

▶ TIME:
- **ns-scale**
  - plasma breakdown
  - ion impacts
- **µs-scale**
  - reaction kinetics
- **ms-scale**
  - mixing rates
- **s-to-∞**
  - electrode aging

<table>
<thead>
<tr>
<th>Length Scales</th>
<th>Time Scales</th>
</tr>
</thead>
<tbody>
<tr>
<td>~ m - device</td>
<td>~ s - electrode aging</td>
</tr>
<tr>
<td>~ mm - turbulence</td>
<td>~ ms - turbulence mixing</td>
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<tr>
<td>~ µm - flame thickness</td>
<td>~ µs - plasma/reaction kinetics</td>
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<tr>
<td>~ µm - plasma sheaths</td>
<td>~ ns - plasma breakdown</td>
</tr>
<tr>
<td>~ nm - chemical reactions</td>
<td>~ ns - plasma breakdown</td>
</tr>
<tr>
<td>~ nm - electrode surface</td>
<td>~ ns - plasma breakdown</td>
</tr>
</tbody>
</table>
A Multi-Character Predictive Science Challenge

- Physics/math character $\Rightarrow$ algorithms $\Rightarrow$ resource utilization

- Hyperbolic
  - Convection: Turbulent mixing

- Elliptic
  - Diffusion: Small-scale, molecular mixing
  - Electric field
  - Radiation

- Atomistic/Particle
  - Electrode damage mechanisms
  - Particle plasma models

- Quantum
  - Electrode work functions
Extreme-Scale Computing Synopsis

► NOW
  - Petascale resources: $10^{15}$ operations/sec
  - Homogeneous: nodes and network
  - Power hungry

► FORECAST (5+ years)
  - Exascale resources: $10^{18}$ operations/sec
  - Ever greater concurrency
  - Heterogeneity
    * more varied specialized processing elements
    * CPUs + GPU-like accelerators + · · ·
    * limited local memory
  - Limited full-system bandwidth
  - More components: more potential faults
  - Input/Output (I/O): costly-to-impractical
  - Power management essential
Use of Exascale ($\times 10^3$ Petascale)

- **Vertical**: $10^3 \times$ more physics
  - more scales
  - increasingly fundamental models
  - $\Rightarrow$ robustness for extrapolation to true prediction

- **Lateral**: $10^3 \times$ more simulations
  - establish input–output statistics:
    - model parameters $\rightarrow$ predictions
  - quantified uncertainty adds predictive value

- Both lead to better Quantity of Interest (QoI) prediction
XPACC: An Exascale-Simulation Problem

► Models can couple reliably only if firmly grounded in physics
  • calibrated sub-models do not guarantee accurate integration
  • represent coupled-physics in detail for low-uncertainty prediction

► Representing physics means, in part, representing length and time scales
  • integrating physics broadens the scale range
  • not computationally additive: depends upon min/max of represented scales

► For low uncertainty, integrating petascale sub-physics models will require exascale

► We will build toward exascale using reduced models, expecting significant-but-quantified initial uncertainty
Exascale-Mapping Predictive Science Challenge

- Different physical models $\Rightarrow$ different discretization $\Rightarrow$ different implementation challenges
- Numerics and implementation design to minimize overhead of mapping onto forthcoming, heterogeneous exascale resources

- General, portable CS advances are necessary to complete this mapping
Exascale: Criteria of Success

• 5-years outlook: trans-petascale/pre-exascale

• Metrics of success toward exascale (and beyond):
  • scale well to levels of concurrency expected in exascale systems
  • scale well in the presence of performance irregularity in computing elements and network
  • perform well, including operations per Joule, with more specialized computing elements and less hardware support
  • produce correct results even in the presence of faults
  • tools must not hinder physics modeling development and simulation
The Team
The Team

Executive Committee

Application Lead
J. Freund (MechSE/AE)

Experimental Lead
G. Elliott (AE)

Principal Investigator/CS Lead
W. Gropp (CS/PCI)

Chief Software Architect
D. Bodony (AE)

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N. Glumac (MechSE)
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Application Simulations
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Max Gunzburger (FSU)
Bob Moser (UT Austin)
Elaine Oran (ONRL)

Chief Software Architect
D. Bodony (AE)
Specific Configuration

- Fuel jet (5 mm; H₂, CH₄) in cross-flow (50 m/s; O₂-Ar, air)
  - A canonical configuration
  - Represents broad class of application configurations
- Plasmas near exit mediate ignition/combustion
  - Spark discharge: radicals and thermal
  - Dielectric barrier discharge: primarily non-thermal via kinetics
- Operate in coupled-physics regime:
  
  \textit{plasma essential for ignition}
Plasma Regime

- Collisional
- Non-thermal: dielectric barrier and nanosecond pulse discharges
- Weakly-thermal/thermal: microsecond pulse discharges
- Temperatures: $T_{n/i} \approx 300 \sim 3000$ K; $\sim 1$ to 10 eV electrons
- Pressure:
  - low ($\sim 50$ Torr) in some calibration experiments
  - higher (1 atm) in target application (practical, rich phenomenology)
- Non-magnetic: Larmor radius $\gg$ mean free path ($r_g = v_\perp/\omega_g \gg \lambda$)
  - Electrostatic: Poisson equation
    $\nabla \cdot (\varepsilon \nabla) \phi = -e(Z_i n_i - n_e)$
Specific Prediction

\[ J(\vec{p}) \]

Adjoint: Gradient
\[ \nabla J = \frac{\partial J}{\partial \vec{p}} \]

- "Find" Burn/No-Burn Boundary
- Identify Key Uncertainties

Burn/No-Burn Boundary
\[ J(\vec{p}) = J_c \]

Parameter Uncertainty
- PDFs from physics-targeted simple-geometry MC assessment

\[ \vec{p} = \{p_1, p_2, \ldots, p_N\} \]

▶ Predict ignition with uncertainty estimate for
- Flow conditions (jet and crossflow)
- Spark operation (kV, duration, rate)
- DBD operation (kV, rate)
Current Status

Compressible flow
LES: Smagorinsky SGS
Hard-coded reduced H₂-air chemistry
Thermomechanically coupled “wall”
Crude heat/radical sources
Current Flow Model

*(Bodony, Freund)*

- Compressible Navier–Stokes
- Reactive mixtures of thermally perfect gases
- Temperature-dependent specific heats

\[
\frac{\partial}{\partial t} \left( \frac{Q}{J} \right) + \frac{\partial F}{\partial \xi} + \frac{\partial G}{\partial \eta} + \frac{\partial H}{\partial \zeta} = \frac{S}{J}
\]

- Solution \(Q\); fluxes \(\{F, G, H\}\); mapping Jacobian \(J\)
- \(S\) source:
  - sub-grid-scale models (large-eddy simulation, ...)
  - chemical/plasma reactions (...)
  - body forces on charged species (...)
  - radiation ‘sink’ (...)
- Coupled with thermo-mechanical (electrode) model
- Validated in hypersonic aerodynamics applications
Year 0 Demonstration Simulation

Air free-stream Mach number $M_\infty$ 0.5
H$_2$ jet Mach number $M_j$ 0.5
Jet diameter $d$ 5 mm
Boundary layer $\delta_{99}$ 5 mm
Reynolds number $Re = \rho_\infty U_\infty d/\mu_\infty$ 46,000

No plasma, reaction, electrodes, $E$-fields, ...
Model Development & Integration

(Pantano, Adamovich, Bodony, Freund, Johnson, Panesi)

Compressible flow
LES: Smagorinsky SGS
Hard-coded reduced H₂- air chemistry
Thermomechanically coupled “wall”
Crude heat/radical sources

Calibrated
2-Reaction Model
Calibrated Phenomenological
Electrode Aging Model
OSU Plasma
Combustion Kinetics
Physics-based
Electrode Aging Model

DFT Work
Functions

DD-LTE-LEE Plasma
SGS Combustion/
Mixing Models
DT Plasma

DS Plasma (f)
SGS Plasma
Transport Models

PMC Plasma

Model Refinement
(and De-refinement)
to Target QoI
Uncertainty

Y0

START

Y1: QoI

Y2: QoI

Y3: QoI

Y4: QoI

Y5: QoI
Spark Discharge Electrodes: Aging

- Spark characteristics depend upon surface details of electrode
- Electrodes age:
  - New
  - 30 Minutes
  - 1 hour
- True predictions will require aging models
- Ion impacts alter mechanical and electronic properties of the electrode surface
  - Roughness focuses electric field, altering ions impacts
  - Damage alters electron work functions, affecting efficacy
Physics-Based Electrode Aging Model

(Johnson, Freund)

- Generalize our time-scale bridging crater-function model
  - MD ion bombardment
  - Statistical response used in continuum model
  - Reproduced ripple-like surface patterns on Si

**INPUT:** Electrode material, geometry, voltage, current

**OUTPUT:** Plasma condition over long damage timescales
Physics-Based Electrode Aging Model

*(Johnson, Freund)*

- Add:
  - Electrostatic alteration of trajectories (build on AFM tip sharpening effort)
  - DFT calculations of electron work functions
    - used extensively to quantify electronic properties of defects and nanostructures: Johnson *et al*.
  - Close interaction with experiments
    - Physics-targeted experiments on electrode aging and its effects
    - Diagnostics of electrode surfaces (e.g. MRL facilities)
  - Build into ‘boundary condition’ for application simulation
Uncertainty Quantification (UQ): Strategy

- Quantified uncertainty increases predictive value
- Quality data and two-way interaction with experiments
  - local experiments designed and refined for UQ objective
  - low-cost, physics-targeted
  - expert quantitative assessment of measurement uncertainties
- Thorough calibration
  - Bayesian inference and sampling
  - fast, low-dimensional, physics-targeted simulations
  - develop and employ model-inadequacy models
  - calibrate models for aleatoric uncertainty (spark discharges)
- Dimensionality reduction
  - sensitivity: remove unimportant uncertain parameter
  - speed: select fidelity for overall QoI uncertainty goals
  - speed: seek surrogates that respect burn/no-burn boundary
- True QoI prediction
  - with quantified uncertainty
  - compared predictively against experiment
UQ: Two-Stage Approach

- Simple configuration, physics-targeted calibration experiments
  - published experimental results
  - designed to emphasize particular physical interactions
  - designed for specific modeling/simulation needs
- Uncertainty propagation to full-system predictions
Physics-Targeted Calibration Experiments

(Elliott, Adamovich, Glumac, Lempert)

Quasi-0D

Plasma-Induced Ignition

Use: plasma models, plasma-coupled ignition kinetics

Status: diagnostic capabilities and flow chamber up and running at OSU (Adamovich, Lempert)
Physics-Targeted Calibration Experiments

(Elliott, Adamovich, Glumac, Lempert)

Quasi-1D

**Plasma-Premixed**

*Use*: plasma ignition validation, quantification of electrode aging and effect, aleatoric modeling of sparks

*Status*: inert analog up and running at Illinois *(Elliott, Glumac)*

**Counterflow Diffusion Flame**

*Use*: kinetics models and effects of augmented radical transport

*Status*: stagnation flow flat-flame variation up and running at OSU *(Adamovich, Lempert)*
Physics-Targeted Calibration Experiments

(Elliott, Adamovich, Glumac, Lempert)

Quasi-2D

**Plasma–Inert Fluid**

*Use:* plasma–flow coupling, quantification of electrode aging and effect; aleatoric model of sparks  
*Status:* zero-flow version up and running at Illinois *(Elliott, Glumac)*

**Plasma-Induced Ignition & Propagation**

*Use:* flame propagation predictions;  
*Status:* diagnostic capabilities and flow chamber up and running at OSU *(Adamovich, Lempert)*
Application / Validation Experiments

(Elliott, Adamovich, Glumac, Lempert)

**Fully 3D**

**Plasma-coupled Burning Turbulent Jet**

*Use:* validation of ignition threshold prediction (and other predictions)

*Status:* tunnel and necessary diagnostics available at Illinois

(Elliott, Glumac)
Overall Roadmap

Geometric Complexity

Year 3 Year 4 Year 2 Year 1 Year 5

+ gnd Prediction UQ Calibration UQ Increasing Sampling

Single Simulation As Physics Models/UQ Necessitates

\[ \text{Ignition} \quad (\sim 0D) \]
\[ \text{Flame} \quad (\sim 2D) \]
\[ \text{Flame kinetics} \quad (\sim 0D) \]
\[ \text{Complex geometry/ turbulence} \quad 3D \]

\[ \text{Model Fidelity} \]

\[ \text{Exascale} \quad \text{Petascale} \quad \text{Terascale} \]

Over-decomposition
Load balancing
Data tiling
Source-to-source

\[ \text{Gamma} \quad \text{G} \quad \text{C} \quad \text{M} \quad \text{M} \quad \text{G} \quad \text{G} \quad \text{G} \quad \text{G} \quad \text{G} \]

GPU acceleration

\[ \text{Prediction UQ} \]
\[ \text{Calibration UQ} \]
\[ \text{Single Simulation} \]
UQ: Calibration

(Freund, Panesi)

- Bayesian inference
  - low-dimensional, physics-targeted experiments
  - fast Monte Carlo parameter calibration simulations

- Priors: select to reflect expectations without restricting range

- Include model-inadequacy model calibration
  (e.g. Kennedy & O’Hagan, 2001; Moser et al. 2012)
QoI Uncertainty

(Freund, Panesi)

- **QoI**: ignition threshold
  - find using adjoint-based gradient

- **Propagate $\vec{p}$ and $\vec{\sigma}$ uncertainty to application predictions**

- **Adjoint-based sensitivity estimate of impact of uncertain parameters on QoI**
  \[
  \sigma_\alpha \frac{\partial J}{\partial p_\alpha}
  \]
  - Eliminate unimportant parametric uncertainties
  - Reduce dimensionality

- **QoI uncertainty: quadrature in uncertainty space**
  - start: sparse, adaptive, MC
  - quantify dependencies and seek surrogates, GP, ...

- **Adjoint: Gradient**
  \[
  \nabla J = \frac{\partial J}{\partial \vec{p}}
  \]
  - "Find" Burn/No-Burn Boundary
  - Identify Key Uncertainties

- **Parameter Uncertainty**
  - PDF's from physics-targeted simple-geometry MC assessment

- **"Find" Burn/No-Burn Boundary**

- **Identify Key Uncertainties**

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- **"Find" Burn/No-Burn Boundary**

- **Identify Key Uncertainties**

- **Adjoint: Gradient**

- **QoI uncertainty: quadrature in uncertainty space**
Adjoint-Based Sensitivity

(Freund, Bodony, Padua)

- Building on experience with adjoint-based control of unsteady, compressible, free shear flows for noise control (AFOSR)
  - Freund et al. (2003,...,2011)
  - Freund & Bodony et al. (2009,...)
Adjoint-Based Sensitivity

(Freund, Bodony, Padua)

- Building on experience with adjoint-based control of unsteady, compressible, free shear flows for noise control (AFOSR)
  - Freund et al. (2003,...,2011)
  - Freund & Bodony et al. (2009,...)

- Developed readily coded exact discrete adjoint for flow-like transport
- Considering a compiler-based approach for general discrete adjoint (Padua)
Example: XPACC in 1D

*(thanks David Buchta)*

- **Goal:** predict ignition (temperature) versus plasma strength
  - Radical addition \((R)\)
  - Plasma heating \((T)\)

- **Physics-targeted experiments → a higher-fidelity model**
  - Reduced \(H_2\)-air mechanism of Boivin et al. (2011)
  - Based on more detailed 21-reaction, 8-species description

### Table 1

<table>
<thead>
<tr>
<th>Reaction</th>
<th>(A^a)</th>
<th>(n)</th>
<th>(E^a)</th>
<th>(A^b)</th>
<th>(n)</th>
<th>(E^b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (H + O_2 \rightarrow OH + O)</td>
<td>(3.52 \times 10^{16})</td>
<td>-0.7</td>
<td>71.42</td>
<td>(7.04 \times 10^{13})</td>
<td>-0.26</td>
<td>0.60</td>
</tr>
<tr>
<td>2 (H_2 + O \rightarrow OH + H)</td>
<td>(5.06 \times 10^{16})</td>
<td>2.67</td>
<td>26.32</td>
<td>(3.03 \times 10^{14})</td>
<td>2.63</td>
<td>20.23</td>
</tr>
<tr>
<td>3 (H_2 + OH \rightarrow H_2O + H)</td>
<td>(1.17 \times 10^{16})</td>
<td>1.3</td>
<td>15.91</td>
<td>(1.28 \times 10^{10})</td>
<td>1.19</td>
<td>78.25</td>
</tr>
<tr>
<td>4 (H + O_2 + M \rightarrow HO_2 + M)</td>
<td>(5.75 \times 10^{16})</td>
<td>-1.4</td>
<td>0.0</td>
<td>(4.65 \times 10^{12})</td>
<td>0.44</td>
<td>0.0</td>
</tr>
<tr>
<td>5 (HO_2 + H \rightarrow 2OH)</td>
<td>(7.08 \times 10^{13})</td>
<td>0.0</td>
<td>1.23</td>
<td>(2.69 \times 10^{12})</td>
<td>0.36</td>
<td>231.86</td>
</tr>
<tr>
<td>6 (HO_2 + H \rightarrow HO_2 + O)</td>
<td>(1.66 \times 10^{13})</td>
<td>0.0</td>
<td>3.44</td>
<td>(2.89 \times 10^{13})</td>
<td>-2.08</td>
<td></td>
</tr>
<tr>
<td>7 (HO_2 + OH \rightarrow HO_2O + O_2)</td>
<td>(1.66 \times 10^{13})</td>
<td>0.0</td>
<td>3.44</td>
<td>(2.89 \times 10^{13})</td>
<td>-2.08</td>
<td></td>
</tr>
<tr>
<td>8 (H + OH + M \rightarrow H_2O + M)</td>
<td>(4.00 \times 10^{22})</td>
<td>-2.0</td>
<td>0.0</td>
<td>(1.03 \times 10^{12})</td>
<td>-1.75</td>
<td>496.14</td>
</tr>
<tr>
<td>9 (2H + M \rightarrow H_2 + M)</td>
<td>(1.30 \times 10^{18})</td>
<td>-1.0</td>
<td>0.0</td>
<td>(1.03 \times 10^{12})</td>
<td>0.0</td>
<td>433.09</td>
</tr>
<tr>
<td>10 (2HO_2 \rightarrow H_2O_2 + O_2)</td>
<td>(3.02 \times 10^{12})</td>
<td>0.0</td>
<td>5.8</td>
<td>(3.04 \times 10^{17})</td>
<td>-0.65</td>
<td></td>
</tr>
<tr>
<td>11 (HO_2 + H_2 \rightarrow H_2O_2 + H)</td>
<td>(1.62 \times 10^{11})</td>
<td>0.61</td>
<td>100.14</td>
<td>(3.04 \times 10^{17})</td>
<td>-0.65</td>
<td>433.09</td>
</tr>
<tr>
<td>12 (H_2O_2 + M \rightarrow 2OH + M)</td>
<td>(8.15 \times 10^{23})</td>
<td>-1.9</td>
<td>207.62</td>
<td>(2.62 \times 10^{19})</td>
<td>-1.39</td>
<td>214.74</td>
</tr>
</tbody>
</table>

*a Units are mol, s, cm³, kJ, and K.

*b Chaperon efficiencies are 2.5 for \(H_2\), 16.0 for \(H_2O\), and 1.0 for all other species; Troe falloff with \(F_c = 0.5\).

*c Chaperon efficiencies are 2.5 for \(H_2\), 12.0 for \(H_2O\), and 1.0 for all other species.

*d Chaperon efficiencies are 2.5 for \(H_2\), 6.0 for \(H_2O\), and 1.0 for all other species;

\[ F_c = 0.265 \exp(-T/94 K) + 0.735 \exp(-T/1756 K) + \exp(-5182 K/T). \]
Example: XPACC in 1D

*(thanks David Buchta)*

- **Goal:** predict ignition (temperature) versus plasma strength
  - Radical addition (R)
  - Plasma heating \((T)\)

- **Physics-targeted experiments \(\rightarrow\) a higher-fidelity model**
  - Reduced \(H_2\)-air mechanism of Boivin *et al.* (2011)
  - Based on more detailed 21-reaction, 8-species description
Example: XPACC in 1D

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▶ Goal: predict ignition (temperature) versus plasma strength
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▶ Physics-targeted experiments → a higher-fidelity model
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  - Based on more detailed 21-reaction, 8-species description

▶ Calibrate simple model:

\[
\begin{align*}
I : & \quad F + O \rightarrow P + R \\
II : & \quad R + M \rightarrow F + M \\
\end{align*}
\]

\[
\begin{align*}
k_I &= A_I T^{n_I} e^{-T/T_i} \\
k_{II} &= A_{II} T^{n_{II}} e^{-T/T_{II}}
\end{align*}
\]
Example: XPACC in 1D

\[ y_k \quad \text{—} \quad T(t = 125 \ \mu s) \quad \text{2-reaction trial predictions} \]
\[ d_k \quad \text{—} \quad T(t = 125 \ \mu s) \quad \text{Boivin et al. ‘data’} \]
\[ T^i_k \quad \text{—} \quad \text{initial temperature for datapoint } k \]
\[ R^i_k \quad \text{—} \quad \text{initial radical concentration (atomic-H in Boivin model)} \]
\[ k \quad \text{—} \quad \text{samples: } k = 1, \ldots, N = 25 \text{ in } \log R^i - \log T^i \text{ plane} \]

▶ Likelihood:

\[
P(\{y_k - d_k\} | \theta, \{R_k, T_k\}, I) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left[ - \frac{\sum (y_k - d_k)^2}{2\sigma^2} \right]
\]

▶ Calibrate \( \theta = \{A_I, A_{II}, n_I, n_{II}, T^a_I, T^a_{II}, \sigma\} \) using Bayesian inference via MCMC
Calibration

\[ n_I, n_{II} \]

\[ T_{II}^a, T_I^a \]
Prediction
Prediction

![Graph showing prediction data with axes labeled \( \log_{10} R_i \) and \( \log_{10} T_i \). The graph includes a color bar indicating temperatures such as 3000K, 2000K, 1000K, 500K, and 200K. There are also histograms on the right side with the temperature \( T \) on the x-axis and the probability density function \( P(T) \) on the y-axis. The peaks of the histograms correspond to the specified temperatures.](image-url)
Prediction

- Challenge at burn/no-burn boundary
- Inadequate model-inadequacy model?
  - single $\sigma$ value
  - biased toward many ‘easy’ predictions away from threshold
- Calibration on joint-PDF (not marginals) essential
  - Marginal PDF yields erroneous, broad, bi-model $T$-prediction due to correlations (e.g. $n_i-T_i$)
Overall Approach Summary

- Data with any associated uncertainty
- Candidate physical model
- Inadequacy model
- Calibrate parameters of both
- Identify important uncertainties for QoI
  - E.g. 0-D calibration → 1-D prediction sensitivities:
    \[
    T_i = 447 \text{ K} \quad R_i = 10^{-3} \quad \sigma_{\text{inad.}} = 48.2
    \]
    \[
    \sigma_{n_i} \frac{\partial J}{\partial n_i} = 20.1 \quad \sigma_{T_i} \frac{\partial J}{\partial T_i} = -33.7 \quad \sigma_{A_i} \frac{\partial J}{\partial A_i} = 6.8
    \]
    \[
    \sigma_{n_{\parallel}} \frac{\partial J}{\partial n_{\parallel}} = 11.1 \quad \sigma_{T_{\parallel}} \frac{\partial J}{\partial T_{\parallel}} = -16.8 \quad \sigma_{A_{\parallel}} \frac{\partial J}{\partial A_{\parallel}} = 0.8
    \]
- Propagate important uncertainty to QoI
- Validation: QoI predicted within combined predicted and data QoI data uncertainty
Summary

▶ Start date…. Jan 1, 2014…
Summary

Start date… Jan 1, 2014… maybe…
Summary

- Start date: Jan 1, 2014... maybe... hopefully
Summary

- Start date.... Jan 1, 2014... maybe... hopefully
  - looking for personnel
Summary

- Start date: Jan 1, 2014... maybe... hopefully
  - looking for personnel

- XPACC is simulation based...
  *predictive science enabled by exascale*
  - bigger simulations: physics faithful across scales
  - more simulations: rigorously integrated for UQ
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▶ XPACC aims to impact combustion beyond its principal PSAAP Predictive-Science goals