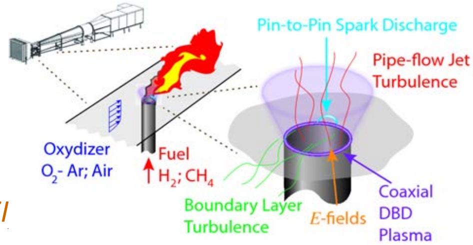
The Center for Exascale Simulation of Plasma-coupled Combustion (XPACC)

Target Applications and Simulation Software

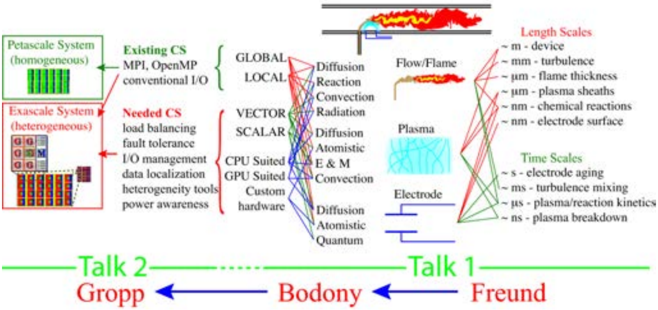


Jonathan B. Freund
Daniel J. Bodony

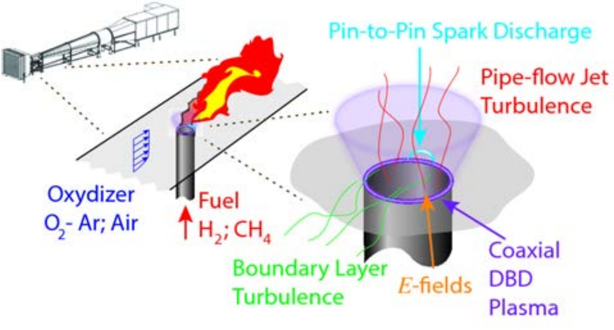
Parallel Computing Institute (PCI
Mechanical Science & Engineerin
Aerospace Engineering

Presentation Plan

- Talk 1: Predictive science goals and plans (Freund)
  - Codebase: exascale enabling algorithms & structure (Bodony)
- Talk 2: Exascale goals and plans (Gropp)

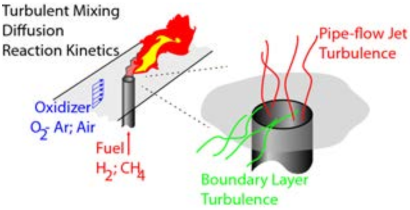


Specific Target Application



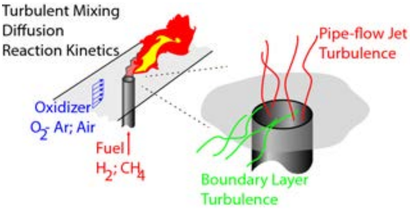
- Predict the ignition threshold of a jet in crossflow via spark-discharge and dielectric-barrier-discharge plasmas
- Canonical combustion flow with new ‘knobs’ for mediating ignition

Combustion



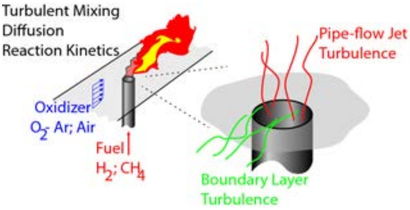
- 'Standard' combustion physics
  - Turbulent mixing
  - Diffusion
  - Fuel-oxidizer determined reaction pathways

Combustion



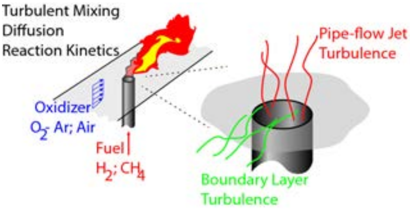
- Engineering design/control:
  - Alter flow rates
  - Alter geometry
  - Alter fuel/oxidizer

Combustion



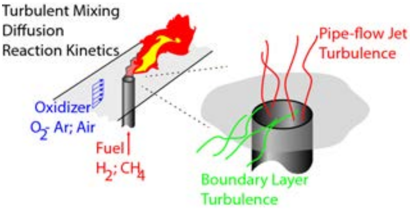
- Engineering design/control:
  - Alter flow rates: application restricted
  - Alter geometry: hard to significantly change residence times
  - Alter fuel/oxidizer: limited availability (*e.g.* air-breathing)

Combustion



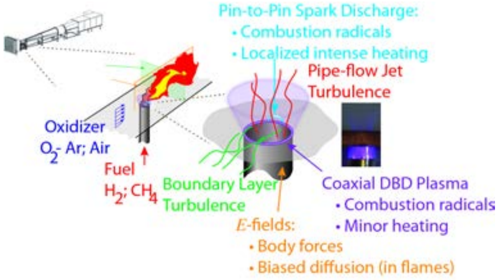
- Indirect control (at most) of key physical mechanism:
  - Reaction kinetics
  - Molecular diffusion
  - Local temperatures

Combustion



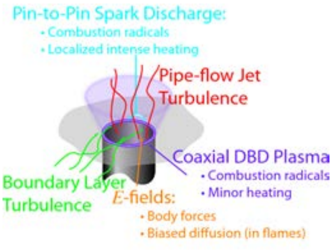
- Indirect control (at most) of key physical mechanism:
  - Reaction kinetics
  - Molecular diffusion
  - Local temperatures
- Plasma-coupling: new multiphysics design 'knobs' for these otherwise inaccessible mechanisms

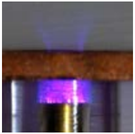
Specific Configuration



- Fuel jet (5 mm; H_2, CH_4) in air cross-flow
- Spark discharge & DBD Plasma
- Operate in coupled-physics regime:
  plasma essential for ignition

Predictive Challenge: Multiphysics

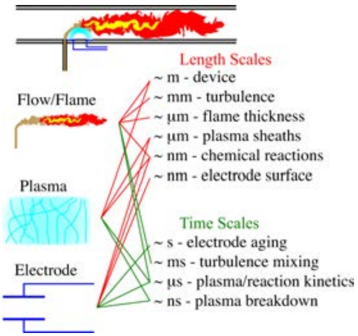




- Plasmas
  - Joule heating: initiates reactions, alters flow via expansion
  - generated radicals 'short-circuit' reaction pathways
- E-fields
  - alter diffusive radical transport: affect thin flame structure
  - force radicals: affects stability even for standard pathways
- Electrodes
  - aging affects spark discharges

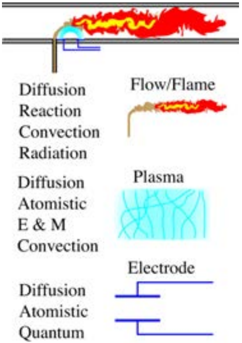
Predictive Challenge: Multiscale

- 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

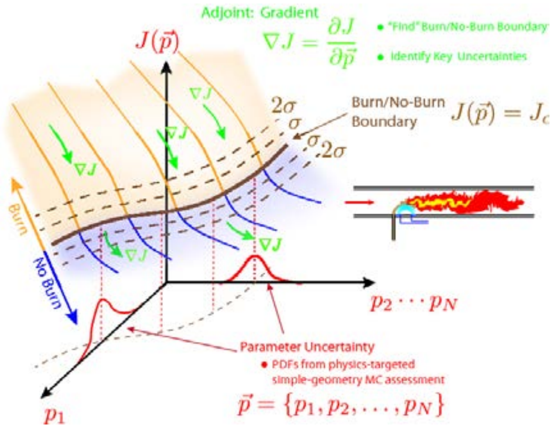


Predictive Challenge: Multicharacter

- Physics/math character ⇒ algorithms ⇒ 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



Specific Prediction

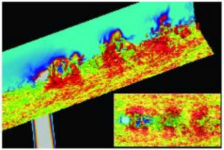


- Predict ignition with uncertainty estimate for
  - Flow conditions (jet and crossflow)
  - Spark operation (kV, duration, rate)
  - DBD operation (kV, rate)

Current Model/Solver

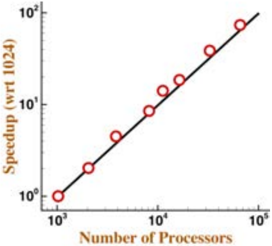
(Bodony, Freund, Pantano)

Compressible flow
LES: Smagorinsky SGS
Hard-coded reduced H_2- air chemistry
Thermomechanically coupled “wall”
Crude heat/radical sources

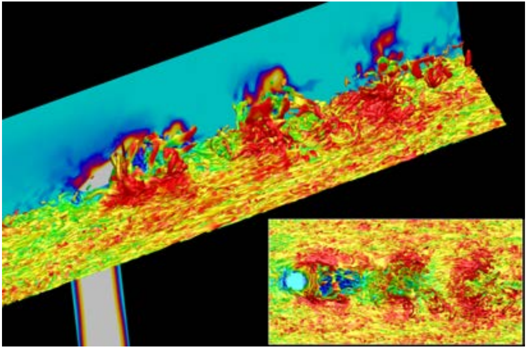


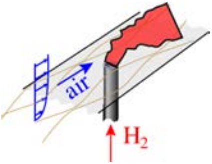
START

- University of Illinois developed
- *PlasComCM*
- Scales to 100K Jaguar CPU cores (blocking operators, single grid)



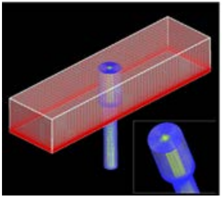
Year 0 Demonstration Simulation





Mesh 1: bound. layer	501 × 106 × 401
Mesh 2: $r \approx 0$	81 × 306 × 81
Mesh 3: cylindrical	161 × 91 × 306

Air free-stream Mach number M_∞	0.5
H_2 jet Mach number M_j	0.5
Jet diameter d	5 mm
Boundary layer δ_{99}	5 mm
Reynolds number $Re = \rho_\infty U_\infty d / \mu_\infty$	46,000

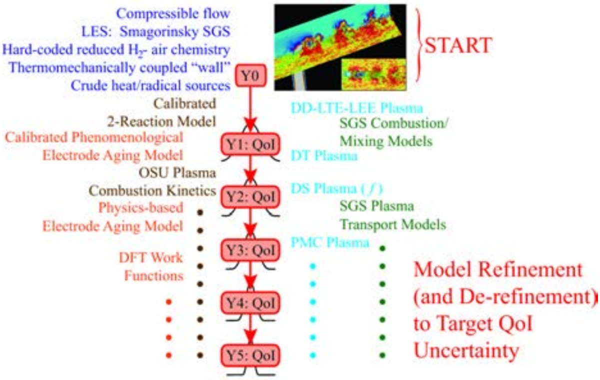


No plasma, reaction, electrodes, *E*-fields, ...

Model Development & Integration

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

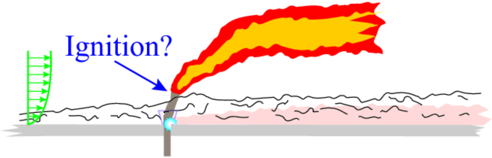
- Models:
  - PDE-fields in turbulence
  - Plasmas
  - Reactions
  - Electrode aging
- Prediction with quantified uncertainty:
  - Approach synopsis
  - Adjoint-based sensitivity
  - Low-D experiments



PDE-Governed Fields

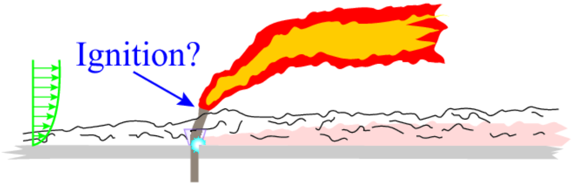
(Pantano, Bodony, Freund)

- DNS & Dynamic SGS turbulence, plasmas, reactions
- Locally-structured tightly coupled overset meshes
- Flexible-order/flexible-resolution finite difference

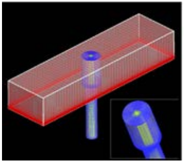


PDE-Governed Fields

(Pantano, Bodony, Freund)

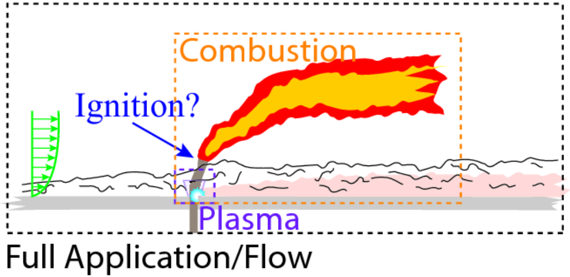


- Start: overset meshes for geometry and spatial resolution needs

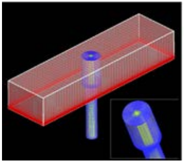


PDE-Governed Fields

(Pantano, Bodony, Freund)

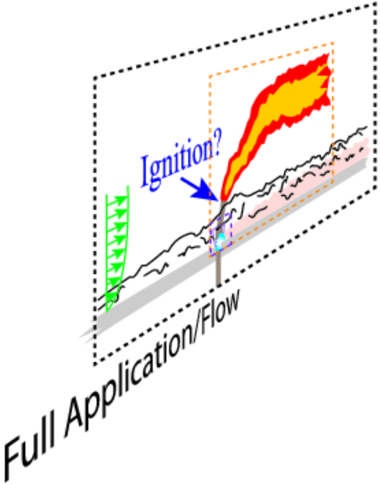


- Start: overset meshes for geometry and spatial resolution needs
- Add: use mesh objects in overset layers for physics-dictated space–time resolution needs



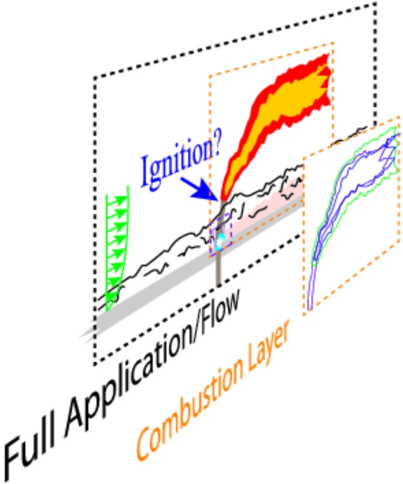
PDE-Governed Fields

(Pantano, Bodony, Freund)



PDE-Governed Fields

(Pantano, Bodony, Freund)



PDE-Governed Fields

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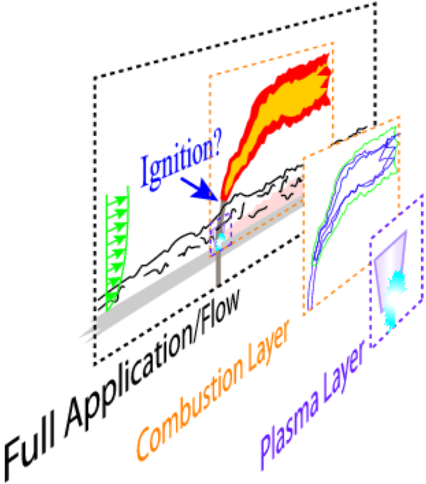


Plasma Model: Description Hierarchy

(Pantano, Panesi, Adamovich)

- Regime: Weakly ionized, non-magnetic
  - Radical production, Joule heating essential for prediction
- Models:
  - Hydrodynamic limits of Boltzmann descriptions
    - Flow-like operators
    - Hierarchy of transport approximations: species (DD), species & fluxes (DT), distributions (DS, *e.g.* Vlasov-Boltzmann)
  - Kinetic:
    - Particle Monte Carlo (*e.g.* PIC methods)
    - 'Break' basic fluid-like operator forms

Plasma-Combustion Kinetics

(Adamovich, Pantano, Panesi)

- Baseline, high-fidelity H_2 kinetics model available
  - Neutrals: N, N_2, O, O_2, O_3, NO, NO_2, N_2O, NO_3
  - Charged: e^-, N^+, N^{+2}, N^{+3}, N^{+4}, O^+, O^{+2}, O^{+4}, NO^+, NO^{+2}, N_2O^+, N_2O^{+2}, N_2NO^+, O_2NO^+, $NONO^+$, O^-, O^{-2}, O^{-3}, NO^-, NO^{-2} , NO^{-3} , N_2O^-
  - Excited: $N_2(A^3\Sigma)$, $N_2(B^3\Pi)$, $N_2(C^3\Pi)$, $N_2(a'^1\Sigma)$, $O_2(a^1\Delta)$, $O_2(b^1\Sigma)$, $O_2(c^1\Sigma)$, $N(^2D)$, $N(^2P)$, $O(^1D)$

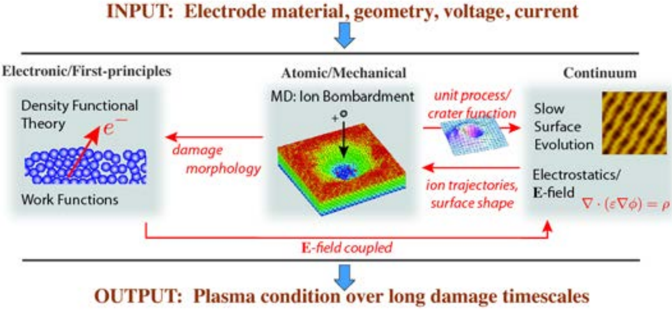
I. V. Adamovich, I. Choi, N. Jiang, J.-H. Kim, S. Keshav, W. R. Lempert, E. Mintusov, M. Nishihara, M. Samimy and M. Uddi, "Plasma assisted ignition and high-speed flow control: non-thermal and thermal effects," *Plasma Sources Sci. Technol.* **18** 034018 (2009).
Y. Zuzeek, S. Bowman, I. Choi, I. Adamovich & W. Lempert, "Pure rotational CARS studies of thermal energy release and ignition in nanosecond repetitively pulsed hydrogen-air plasmas," *Proc. Comb. Inst.* **33** 3225 (2011).
N. A. Popov "Effect of a pulsed high-current discharge on hydrogen-air mixtures," *Plasma Physics Reports* **34**, 376 (2008).

- Develop, improve, UQ-calibrate for plasma conditions

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 surface patterns & FIB milling
- DFT: damage effect on electron work function



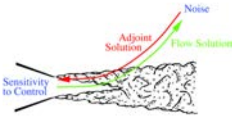
Quantifying Uncertainty

(Freund, Panesi)

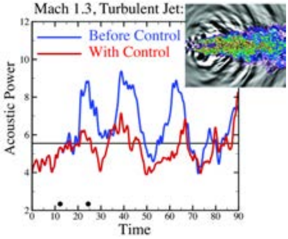
- Quality data and two-way interaction with experiments
  - local experiments designed and refined for UQ objective
  - low-cost, physics-targeted
  - expert quantitative assessment of measurement uncertainties
- Thorough calibration
  - Bayesian inference and sampling
  - fast, low-dimensional, physics-targeted 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

Adjoint-Based Sensitivity

(Freund, Bodony)

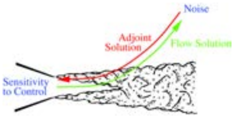


- Building on experience with adjoint-based control of unsteady, compressible, free shear flows for noise control (AFOSR)
  - Freund *et al.* (2003,...,2011)
  - Freund & Bodony *et al.* (2009,...)



Adjoint-Based Sensitivity

(Freund, Bodony)



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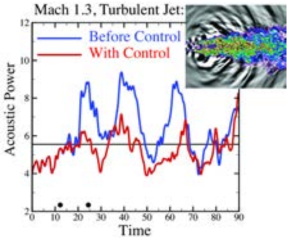
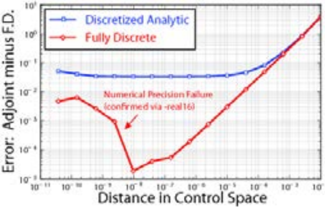




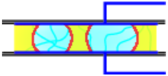
- Developed readily coded exact discrete adjoint for flow-like transport

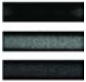
Physics-Targeted Calibration Experiments

(Elliott, Adamovich, Glumac, Lempert)

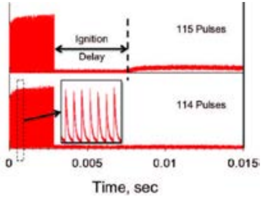
Quasi-0D

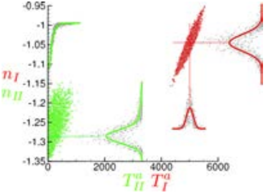
Plasma-Induced Ignition

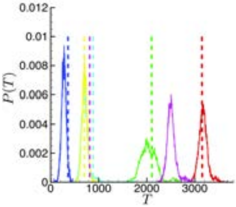




Use: plasma models, plasma-coupled ignition kinetics **Status:** diagnostic capabilities and flow chamber up and running at OSU *(Adamovich, Lempert)*





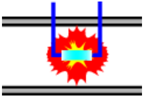


Physics-Targeted Calibration Experiments

(Elliott, Adamovich, Glumac, Lempert)

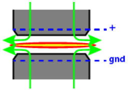
Quasi-1D

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



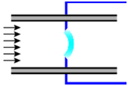
Use: kinetics models and effects of augmented radical transport; **Status:** stagnation flow flat-flame variation up and running at OSU *(Adamovich, Lempert)*

Physics-Targeted Calibration Experiments

(Elliott, Adamovich, Glumac, Lempert)

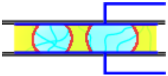
Quasi-2D

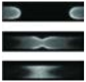
Plasma–Inert Fluid



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





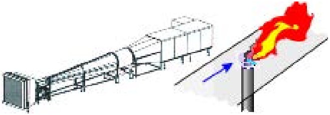
Use: flame propagation predictions; **Status:** diagnostic capabilities and flow chamber up and running at OSU *(Adamovich, Lempert)*

Application / Validation Experiments

(Elliott, Adamovich, Glumac, Lempert)

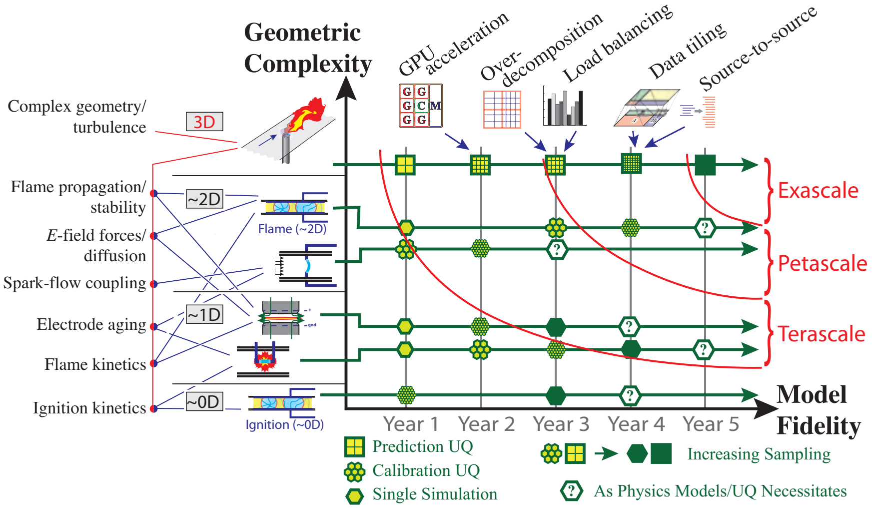
Fully 3D

PLASMA-COUPLED TURBULENT JET IGNITION



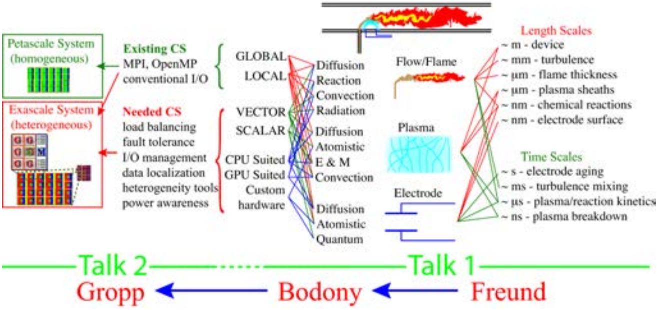
Use: validation of ignition threshold prediction (and other predictions) **Status:** tunnel and necessary diagnostics available at Illinois *(Elliott, Glumac)*

Overall Roadmap



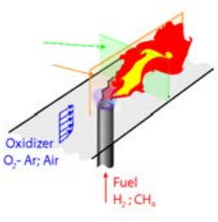
Toward Exascale

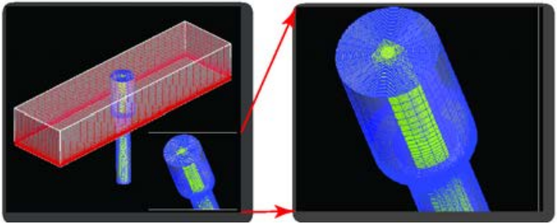
- Predictive science effort built on Illinois *PlasComCM*
- Operator structure:
  - flexible discretization (*e.g.* high-/low-order) as best for physics
  - geometry: locally structured, globally unstructured
  - facilitate co-development of physics discretization and exascale enabling tools



PlasComCM: Overset Grids

Space: locally structured—globally unstructured. . .

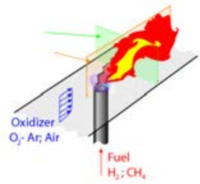




. . . which brings several advantages:

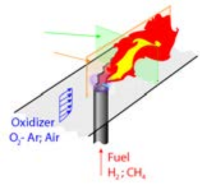
- Straightforward adaptivity (multiresolution, variable sencils)
- Natural asynchrony (multi-timestepping, concurrency, scheduling for latency hiding)
- Variable-order (soft error checking, Poisson preconditioning)
- Lightweight, simple data structures (tiling, runtime control)

PlasComCM: Operators



- Physical models: $\partial/\partial t$, $\partial/\partial x_i$, $\partial^2/\partial x_i \partial x_j$, ∇^{-1}, $\iint f_{\text{col}}(\theta, \phi)\, \mathrm{d}\theta \mathrm{d}\phi$

PlasComCM: Operators



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- Exascale access: speed, memory locality, scability, power usage, cache blocking, ...

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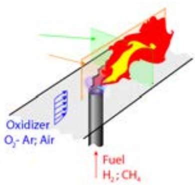

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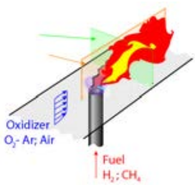
Operators unify these two sets of needs:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} + f(u) \quad \underset{\{x_i\}_{i=1}^N}{\overset{\text{disc.}}{\Longrightarrow}} \quad \frac{\mathrm{d}\vec{u}}{\mathrm{d}t} = -aD_x\vec{u} + \nu D_{xx}\vec{u} + F[\vec{u}]$$

- The models care about $D_{[x|xx]}\vec{u}$ while the CS exascale tools care about $D_{[x|xx]}$

PlasComCM: Operators



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- The models care about $D_{[x|xx]}\vec{u}$ while the CS exascale tools care about $D_{[x|xx]}$
- Code separates out the use of an operator from its declaration...

Operators—Declaration (Stencil Based)

$$D = \begin{bmatrix} \times_L & \times_L & \times_L & \times_L & \times_L & 0 & 0 & 0 & 0 \\ \times_L & \times_L & \times_L & \times_L & \times_L & 0 & 0 & 0 & 0 \\ \times_I & \times_I & \times_I & \times_I & \times_I & 0 & 0 & 0 & 0 \\ 0 & \times_I & \times_I & \times_I & \times_I & \times_I & 0 & 0 & 0 \\ 0 & 0 & \times_I & \times_I & \times_I & \times_I & \times_I & 0 & 0 \\ 0 & 0 & 0 & \times_I & \times_I & \times_I & \times_I & \times_I & 0 \\ 0 & 0 & 0 & 0 & \times_I & \times_I & \times_I & \times_I & \times_I \\ 0 & 0 & 0 & \times_R & \times_R & \times_R & \times_R & \times_R & \times_R \\ 0 & 0 & 0 & \times_R & \times_R & \times_R & \times_R & \times_R & \times_R \end{bmatrix} = \begin{bmatrix} D_L \\ D_I \\ D_R \end{bmatrix}$$

Operators—Declaration (Stencil Based)

$$D = \begin{bmatrix} D_L \\ D_I \\ D_R \end{bmatrix} \qquad D\vec{f} = \begin{bmatrix} D_L \\ \cdot \\ \cdot \end{bmatrix} \begin{bmatrix} \vec{f}_L \\ \cdot \\ \cdot \end{bmatrix} + \begin{bmatrix} \cdot \\ \cdot \\ D_R \end{bmatrix} \begin{bmatrix} \cdot \\ \cdot \\ \vec{f}_R \end{bmatrix} + \begin{bmatrix} \cdot \\ D_I \\ \cdot \end{bmatrix} \begin{bmatrix} \cdot \\ \vec{f}_I \\ \cdot \end{bmatrix}$$

- L, R, and I parts independent $\Longrightarrow$ scheduling
- Sparsity patterns known and different $\Longrightarrow$ separate algorithms for L, R vs. I; prefetching hints; streaming
- Permit tiling, threads, data layout for efficient memory utilization

Operators—Use (Stencil Based)

Consider active scalar equation (in 2-D)

$$\frac{\partial \rho Y_i}{\partial t} = -\frac{\partial}{\partial x_j}\left[\rho(u_j + V_j^i)Y_i\right] + S_i(\rho, T, Y_j)$$

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- Application user requests tasks with dependency hints

```
for(i = 0; i < Ns; i++) {
     rhs(:,i) = 0;
     rhs(:,i) += ApplyOperator(D_x,-cv(:,1)*(u(:,1) + V(:,i,1))*Y(:,i),ASYNC);
     rhs(:,i) += ApplyOperator(D_y,-cv(:,1)*(u(:,2) + V(:,i,2))*Y(:,i),ASYNC);
     rhs(:,i) += ApplyOperator(S_i,[rho T Y],ASYNC);
     WaitOperators();
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Operators—Use (Stencil Based)

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```
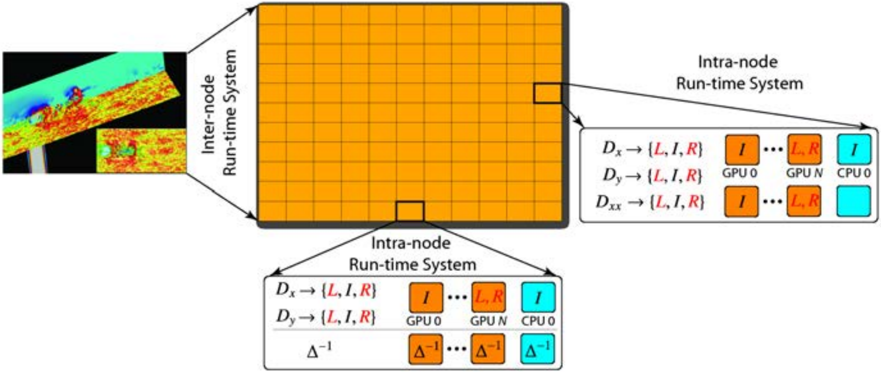
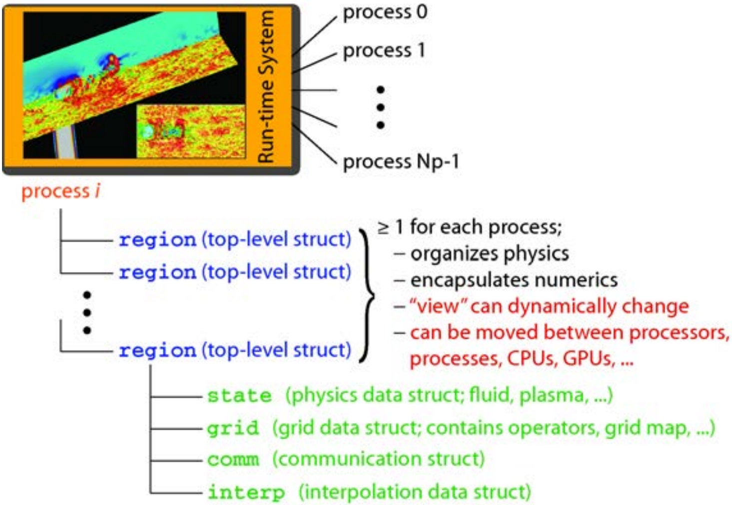

- Research issues: memory motion, data layout management, scheduling, ...
- Code transformations can be done to code within `ApplyOperator`
- "Golden Copy" code always available

Operators and the Runtime System



Key message: Operators yield flexibility

Flexible Datastructures



Path to Exascale

- High-level operator-based abstraction (ANSI C/F90)
- Natural multiscale (overset) & asynchrony
- Good (pre-)petascale scaling
- Flexible datastructures, object-oriented, flexible order
- Lightweight language, easy to capture action of operators
- Built for on-the-fly adaptation (e.g., Charm++ runtime)
- Data layout can be changed
- Demonstrated CPU-GPU integration
- Proven code structure for developing multiphysics simulations

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$\Longrightarrow$ Ready for Year 1 simulations and exascale tools (Talk 2)