



# SIMCENTER

NATIONAL CENTER  
*for* COMPUTATIONAL  
ENGINEERING

Overview

Dr. Henry McDonald

***Presented by Dr. Kyle Anderson***

*February 11, 2008*



## VISION

*To be the best computational engineering research and education center in the world.*

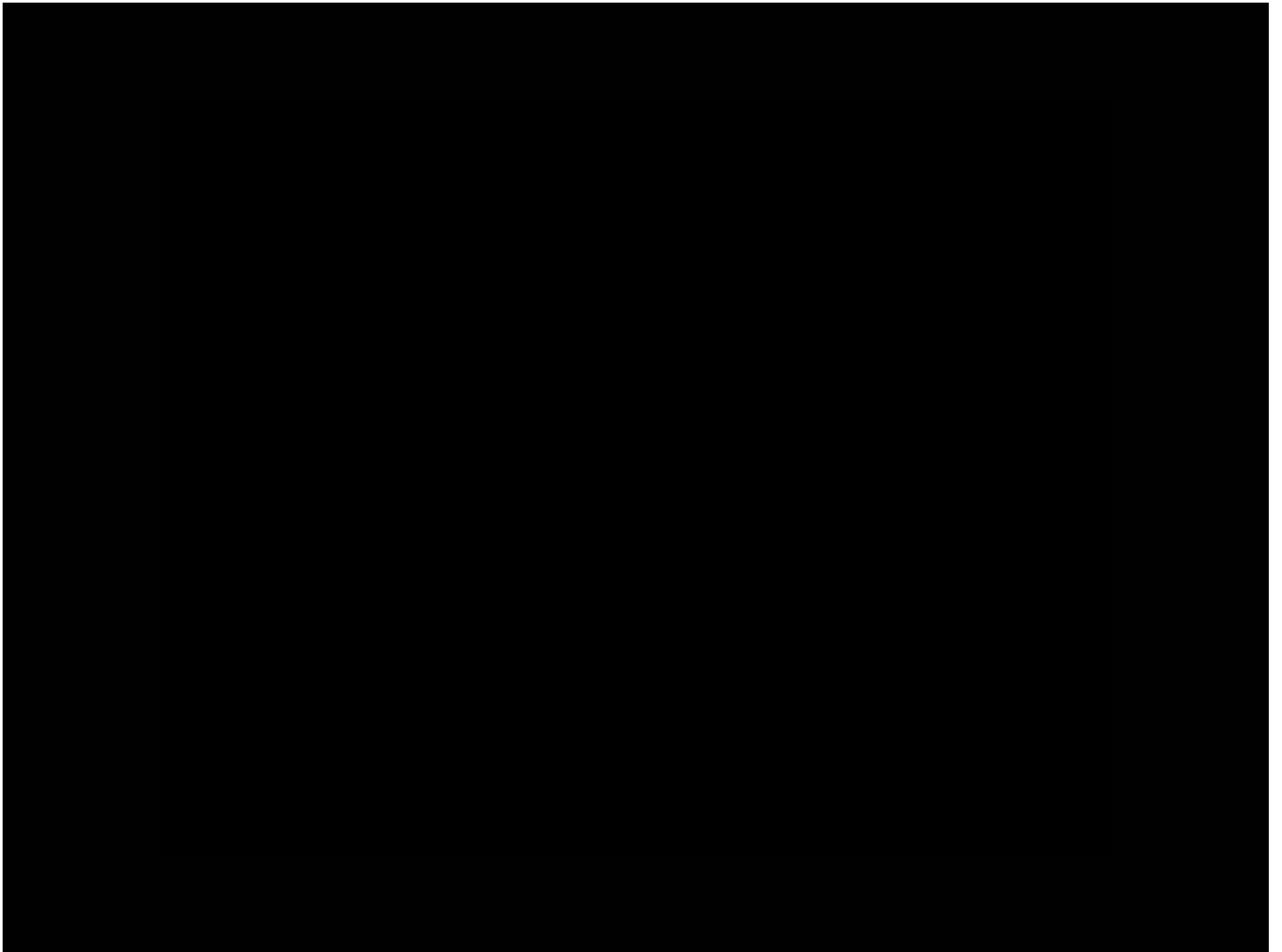
## MISSION

*To support U.S. global competitiveness and regional economic development through integrated research and education in computational engineering.*

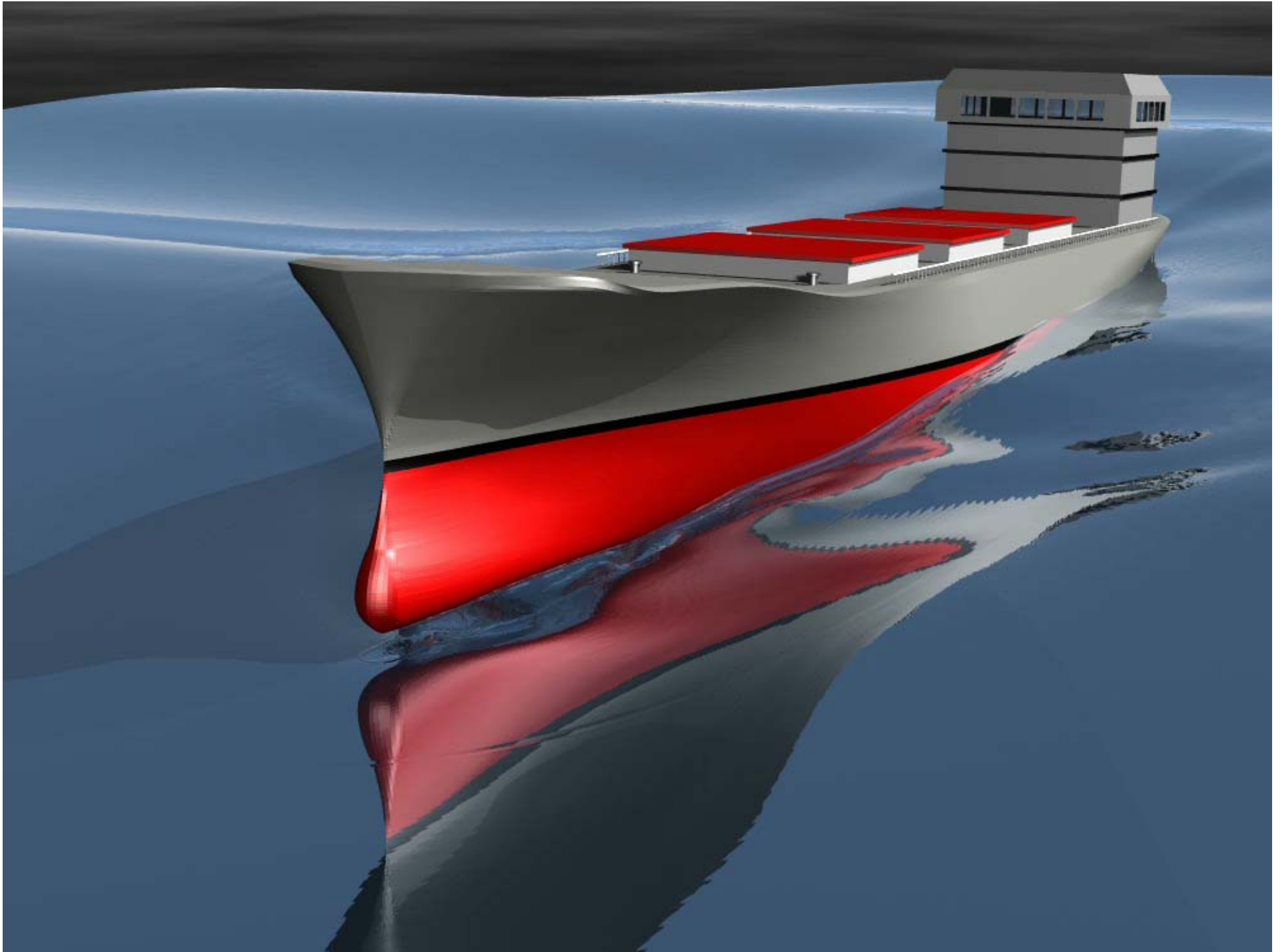
# What is Computational Engineering?

***An emerging multidiscipline that solves complex, practical, real-world engineering analysis and design problems using advanced computer simulations based on physical and mathematical models***



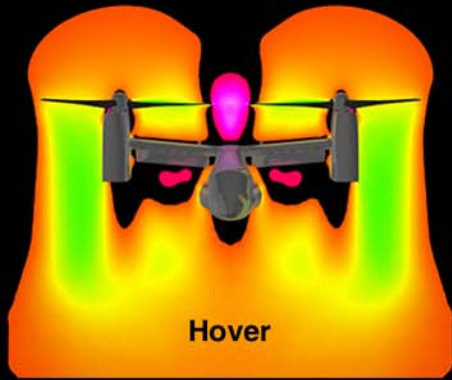






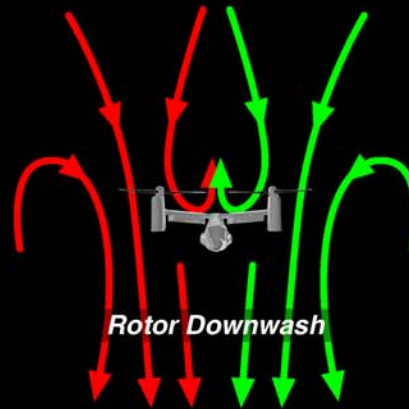
# Forensic Engineering



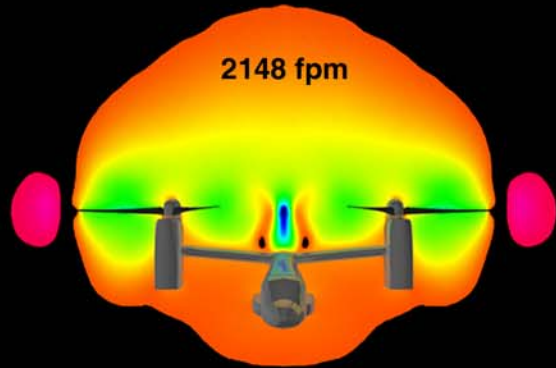


Hover

Rotor Downwash Generates Lift During Hover

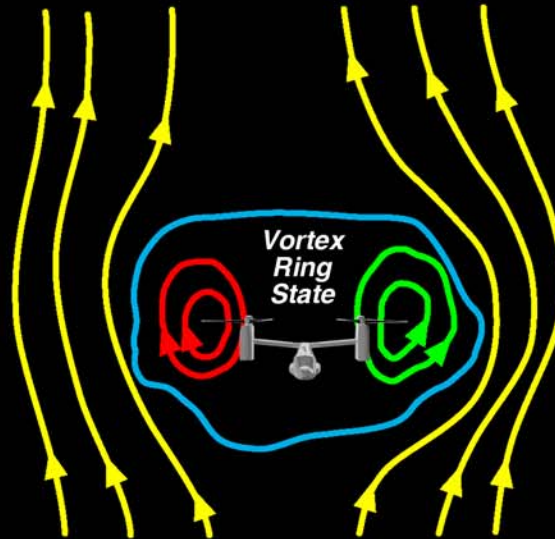


Rotor Downwash



2148 fpm

Loss of Lift Occurs at Large Vertical Descent Velocity



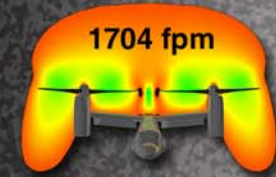
Vortex Ring State

Instantaneous Vertical Velocity

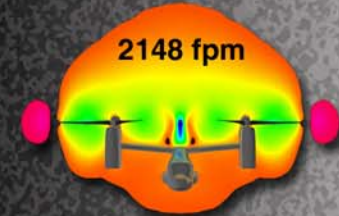


-0.5

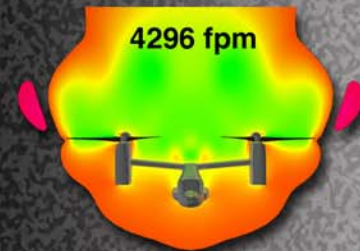
0.2



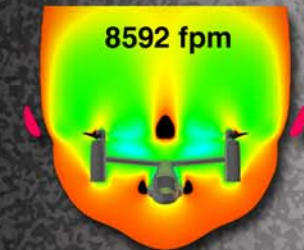
1704 fpm



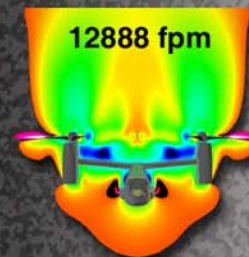
2148 fpm



4296 fpm



8592 fpm

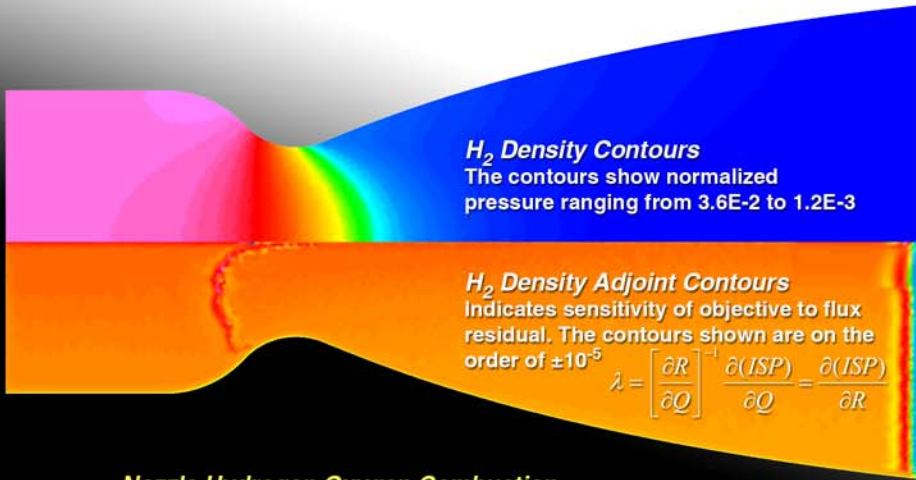


12888 fpm

Other Descent Rates

# Loss of Rotor Lift at Large Descent Velocity

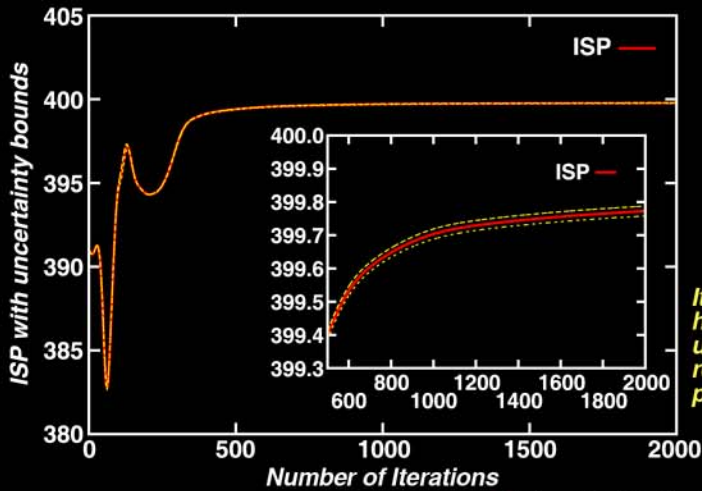




**Nozzle Hydrogen Oxygen Combustion**

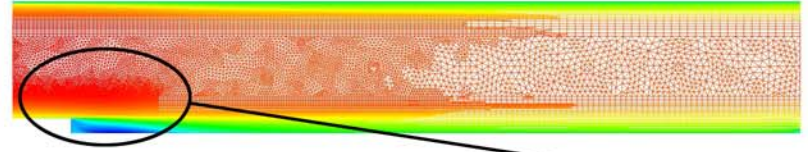
Reaction equation	$\beta = \eta f$	$ \Delta\beta $	$ dISP/d\beta $	$ \Delta ISP $
2O+M $\rightleftharpoons$ O <sub>2</sub> +M	-1	1.00E-01	2.73E-08	4.50E-07
2H+H <sub>2</sub> $\rightleftharpoons$ 2H <sub>2</sub>	-0.6	6.00E-02	9.31E-06	9.22E-05
2H+H <sub>2</sub> O $\rightleftharpoons$ H <sub>2</sub> +H <sub>2</sub> O	-1.25	0.125	9.15E-05	1.89E-03
O+H+M $\rightleftharpoons$ OH+M	-1	0.1	2.39E-06	3.94E-05
H+OH+M $\rightleftharpoons$ H <sub>2</sub> O+M	-2	0.2	3.36E-04	1.11E-02
H+O <sub>2</sub> $\rightleftharpoons$ O+OH	-6.707	0.6707	1.62E-05	1.80E-03
O+H <sub>2</sub> $\rightleftharpoons$ H+OH	2.7	2.70E-01	6.28E-07	2.80E-05
2OH $\rightleftharpoons$ O+H <sub>2</sub> O	2.4	2.40E-01	1.17E-07	4.65E-06
OH+H <sub>2</sub> $\rightleftharpoons$ H+H <sub>2</sub> O	1.51	0.151	1.12E-06	2.79E-05

Baseline ISP: 399.81  
Total  $|\Delta ISP|$ : 1.50E-02

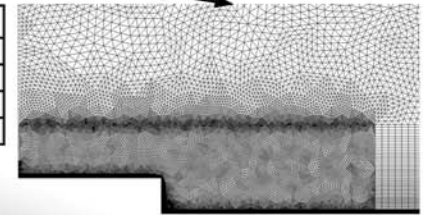


Iterative history including uncertainty due to reaction-rate parameters

Final adapted mesh constructed from output-based adaptation method (aggressive adaptation tolerance due to high aspect ratio boundary elements)



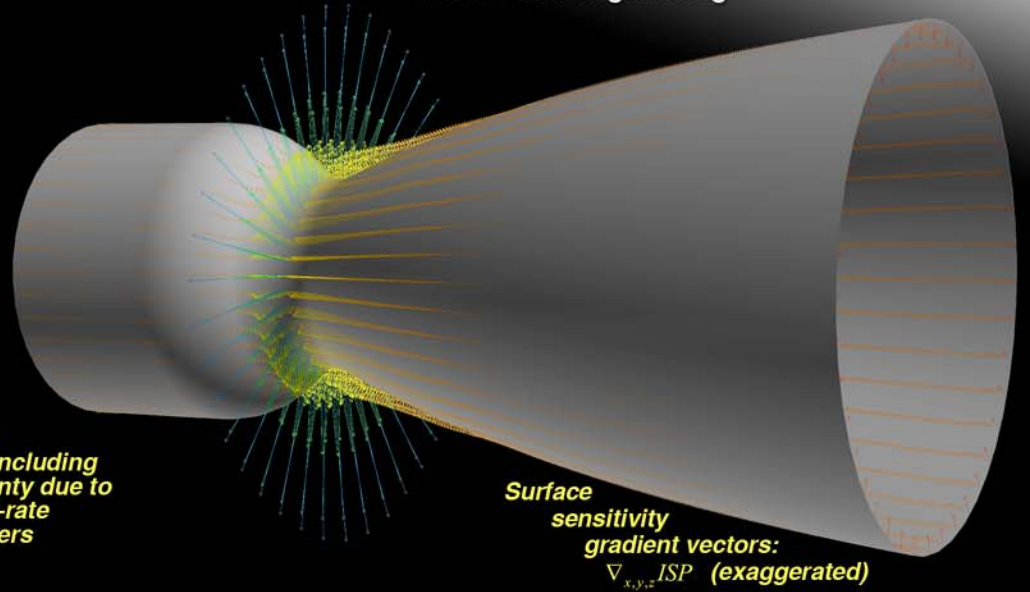
Model	Xr	Total $ \Delta Xr $
Spalart	7.71E+00	5.63E-01
q- $\omega$	7.11E+00	1.66E+00
k- $\epsilon$	6.56E+00	3.15E-04
Experiment*	7.00E+00	1.00E+00



Close-up of mesh resolution near backstep

**Adjoint-Based Grid Adaptation/Sensitivity Analysis**

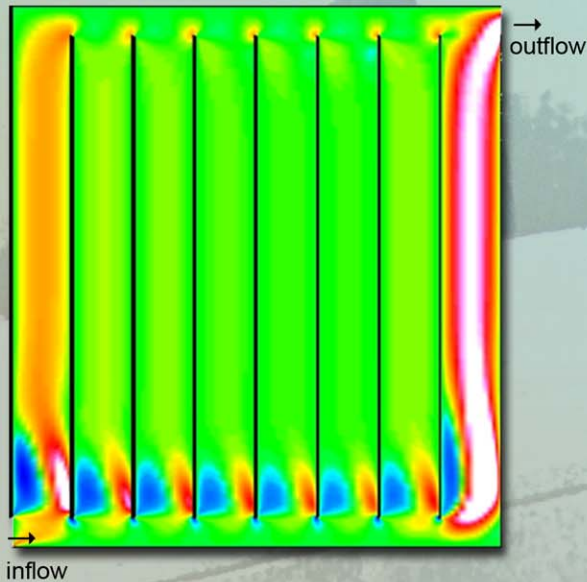
Sponsored by: The Tennessee Higher Education Commission  
Center of Excellence for Applied Computational Science and Engineering



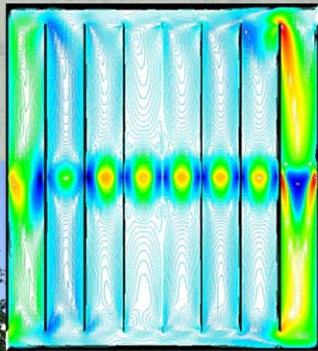
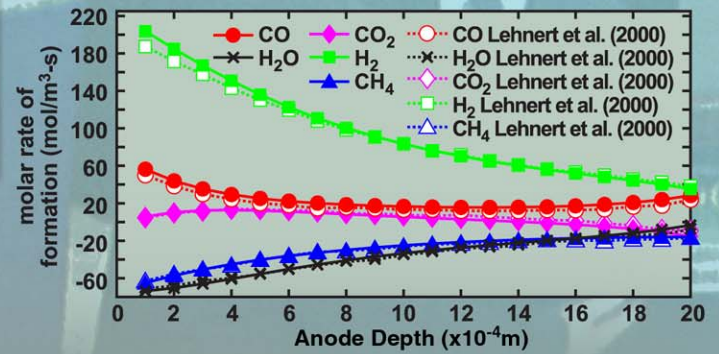
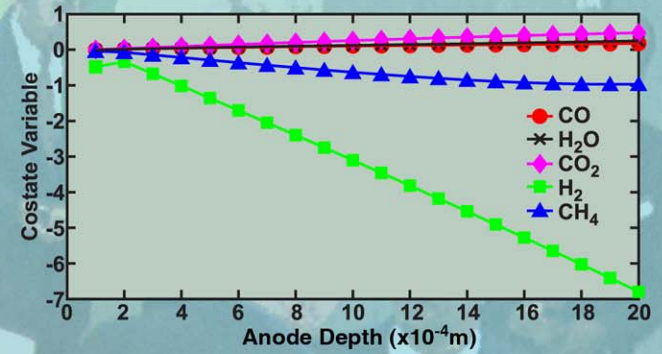
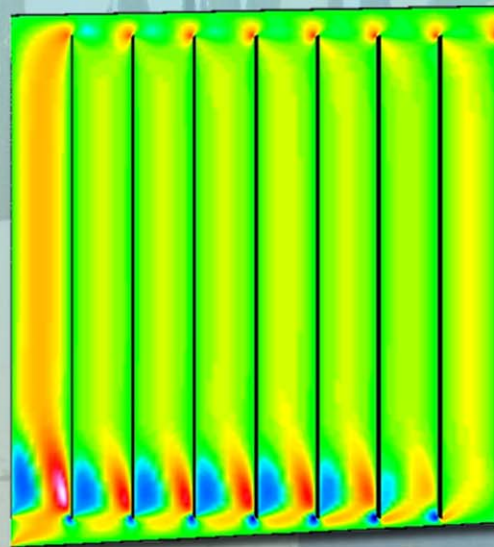
\*Eaton, J.K., Johnston, J.P., "A Review of Research on Subsonic Turbulent Flow Reattachment," AIAA Journal, Vol. 19, No. 9, September 1981. AIAA-80-1438



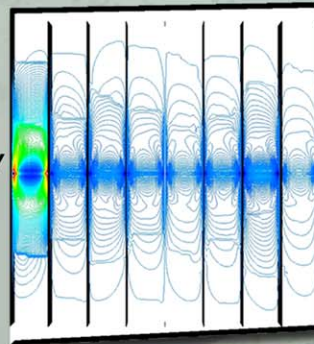
Fuel Distribution Before Reshaping



Fuel Distribution After Reshaping



Flow Sensitivity Contours



**Notional Solid-Oxide Fuel Cell Sensitivity/ Design Study**

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Center of Excellence for Applied Computational Science and Engineering and the Department of Energy

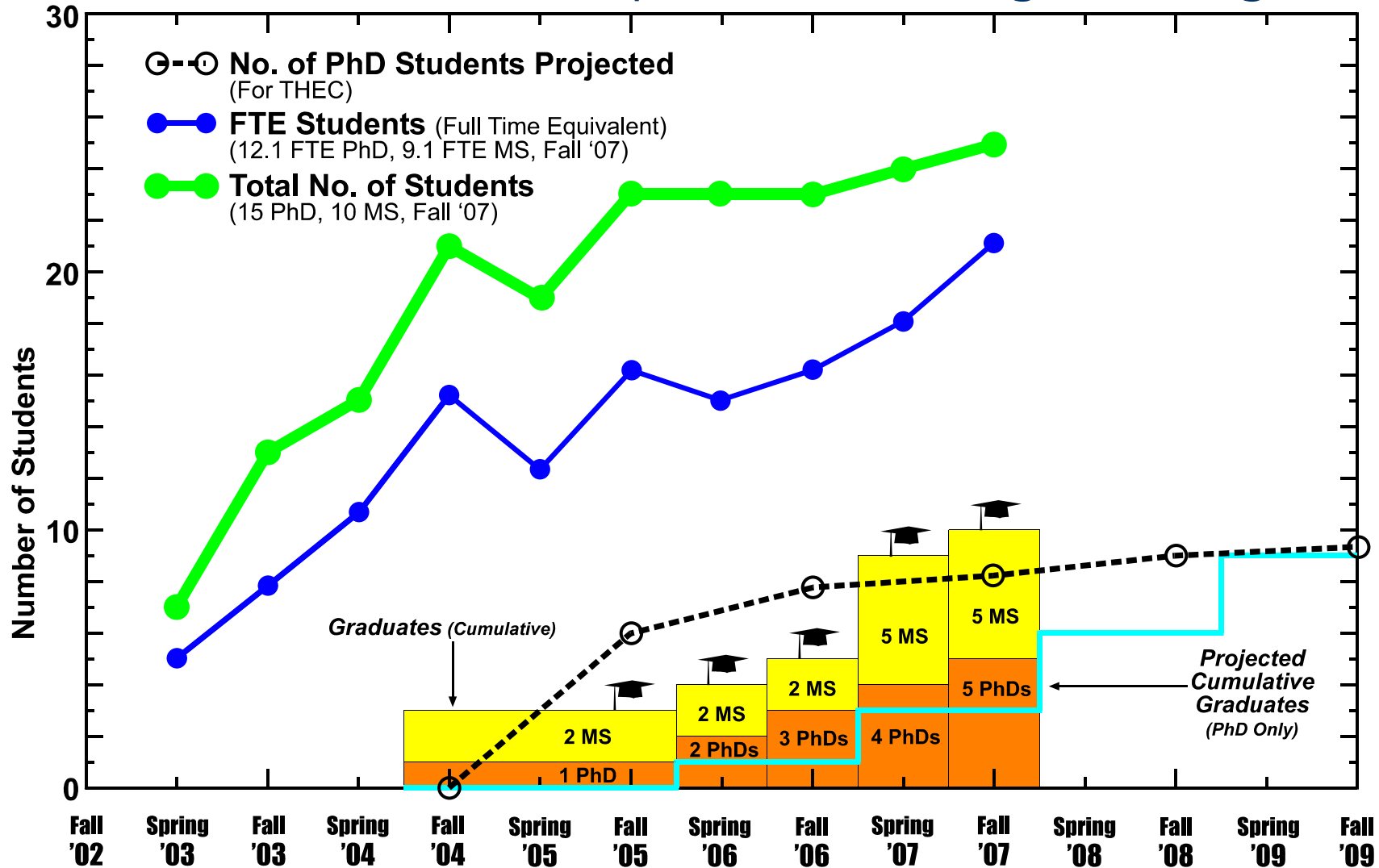


U.S. Congressman Zach Wamp (L) and UTC Chancellor Roger Brown (R) at the dedication ceremony for the Alternative Energy Laboratory held on February 17, 2006.

	Cost Function – Molar Concentration of Hydrogen at Anode-Electrolyte Interface		
	$dI/da_t$	$dI/d\psi$	$dI/d\langle r \rangle$
Design Variable	$a_t$ – Anode Thickness	$\psi$ – Porosity/Tortuosity	$\langle r \rangle$ – Mean Pore Radius
Finite Differences	3.0103686566e-01	-1.0500656390e-03	-7.2445001109e+01
Adjoint	3.0103704637e-01	-1.0500656734e-03	-7.244506333e+01

Comparison of sensitivity derivatives obtained using the adjoint method with those obtained using finite differences.

# Students in Computational Engineering



# The SimCenter Today:

**Research Team:** *22 Academic and Research Faculty and Staff*

**M.S. and Ph.D. in Computational Engineering**  
*25 Ph.D and M.S. Students*

**Doctoral Program established in 2004**  
**Graduated 5 M. S. and 5 Ph.D. Students to Date**

**\$16.6 Million in external research contracts**

***“The SimCenter is the most advanced computational modeling and simulation center in the nation, with outstanding teaching and research faculty ...”***

***- THEC External Review***



# The Next Step



## **Expansion**

*Goal of 100 faculty and 100 graduate students*

# How Will It Work?

- Modeled After the University of Tennessee SimCenter at Chattanooga
- Interdisciplinary Team of Professionals and Students Engaged in Application Driven Research
- Tools Would be Large, Dedicated, Advanced Supercomputers and Advanced Communication Systems





Private Sector Commits  
Over \$17 Million

***Lyndhurst Foundation***

***Benwood Foundation***

***UC Foundation***

***Maclellan Foundation***

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UTC SimCenter  
November 20<sup>th</sup>, 2007