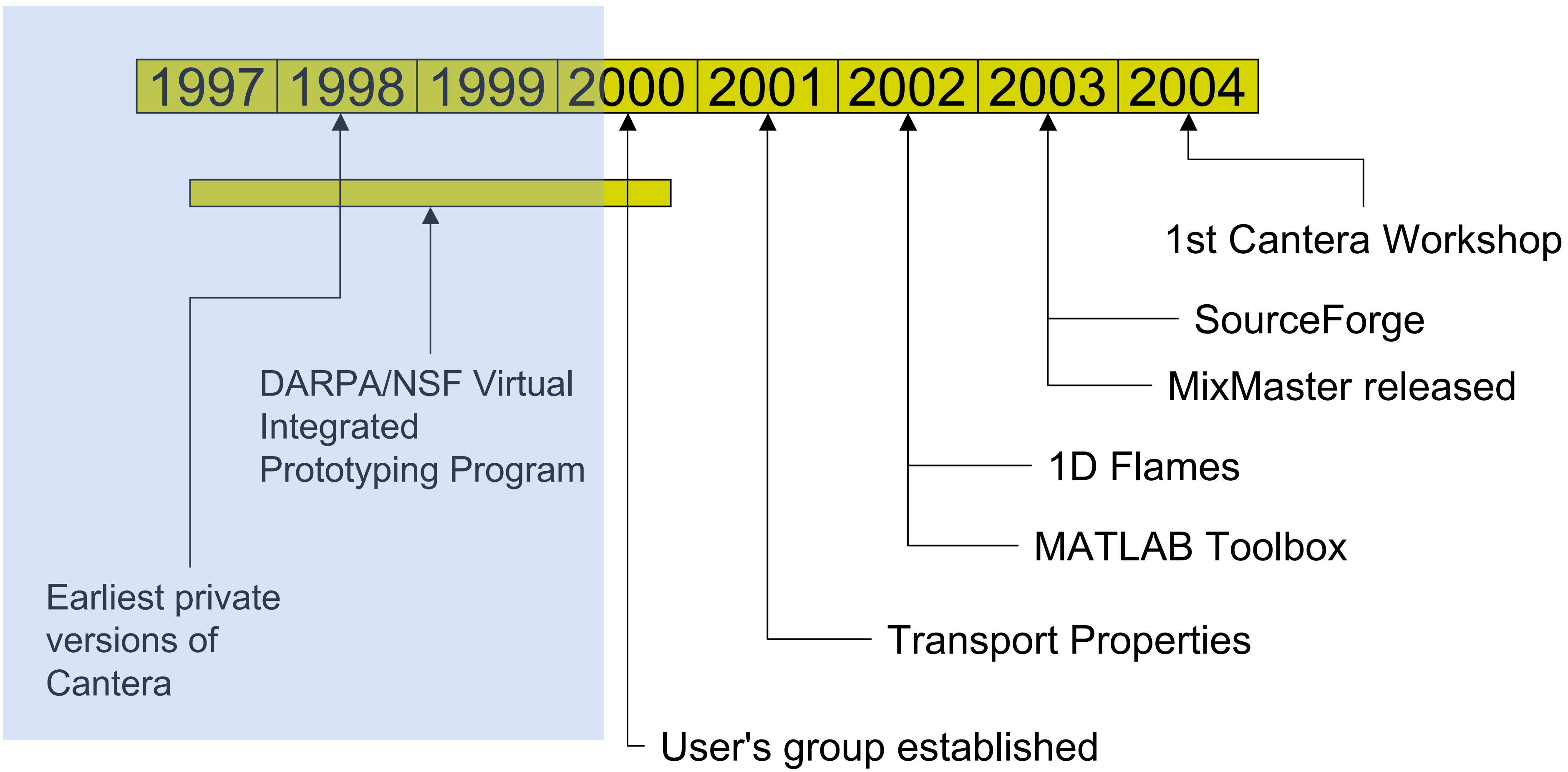
Cantera Workshop

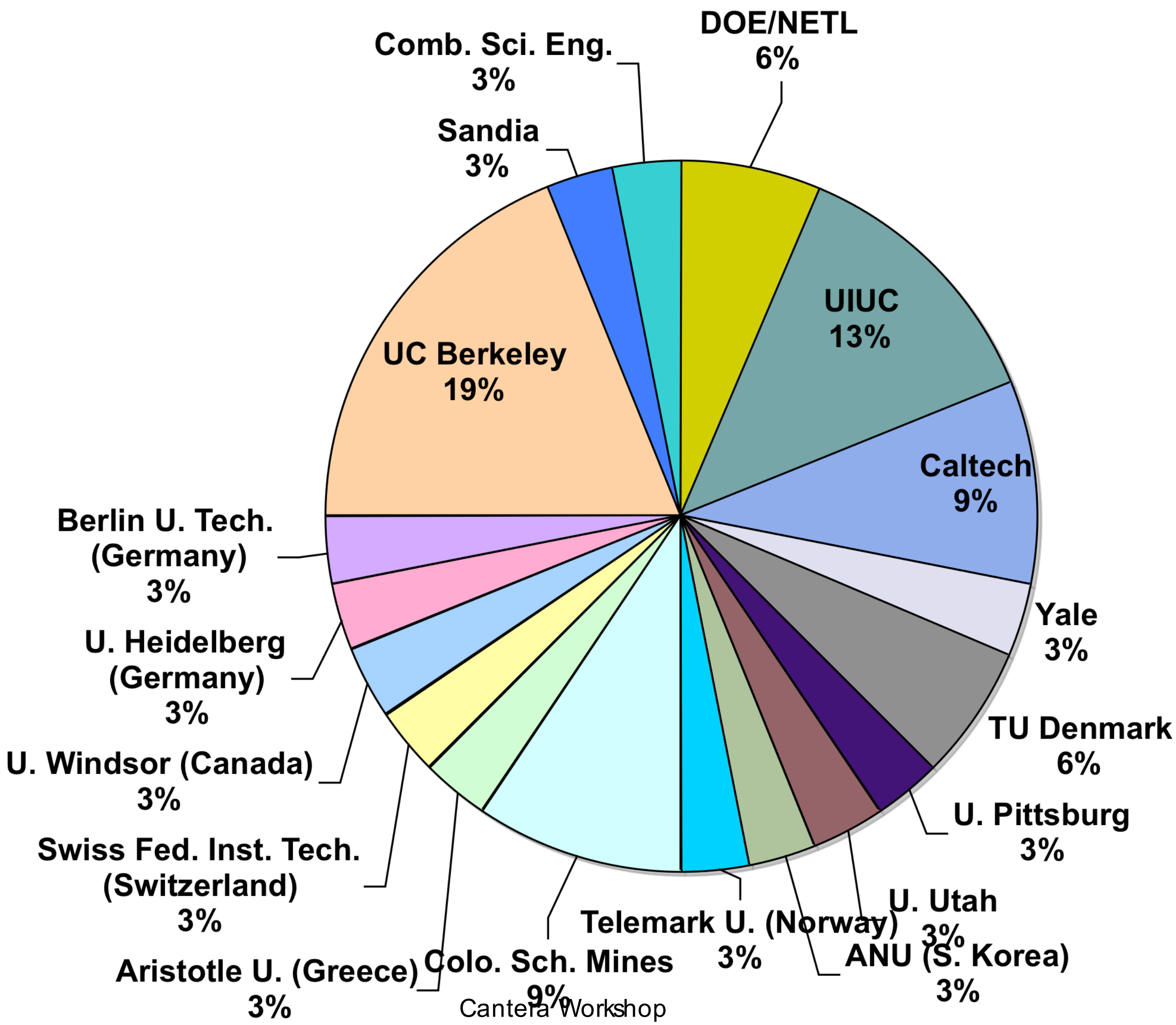
Welcome to the First Workshop
on Cantera!

Timeline



1997
1998
1999
2000
2001
2002
2003
2004
1st Cantera Workshop
SourceForge
MixMaster released
1D Flames
MATLAB Toolbox
Transport Properties
User's group established
DARPA/NSF Virtual Integrated Prototyping Program
Earliest private versions of Cantera

Preregistered Workshop Attendees



Agenda

9:00	D. Goodwin	Introduction to Cantera
9:20	D. Goodwin	Defining and Using Phases and Interfaces
9:50	D. Goodwin	Reactor Networks
10:15	Dibble, Mack, Mehresh, and Chen, UCB	20 Homework Problems in Combustion using MATLAB Cantera
10:40		Break
11:00	D. Goodwin	One-Dimensional Flame Simulations
11:30	C. Pantano Caltech	Using Cantera to Construct Flamelet Libraries for Large-Eddy Simulation
12:00		Lunch
1:00	D, Goodwin	Cantera C++ Programming
1:20	E. D. Huckaby, DOE/NETL	Extending Cantera
1:40	E. D. Huckaby, DOE/NETL	Coupling Cantera to Fluent
2:00		Discussion / Future directions

Introduction to Cantera

David G. Goodwin

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Applied Science
California Institute of Technology

Cantera is a set of software tools for problems involving kinetics

Some Capabilities:

- Thermodynamic properties
- Transport properties
- Chemical equilibrium
- Homogeneous and heterogeneous chemistry
- Reactor networks
- One-dimensional flames
- Electrochemistry
- Reaction path diagrams

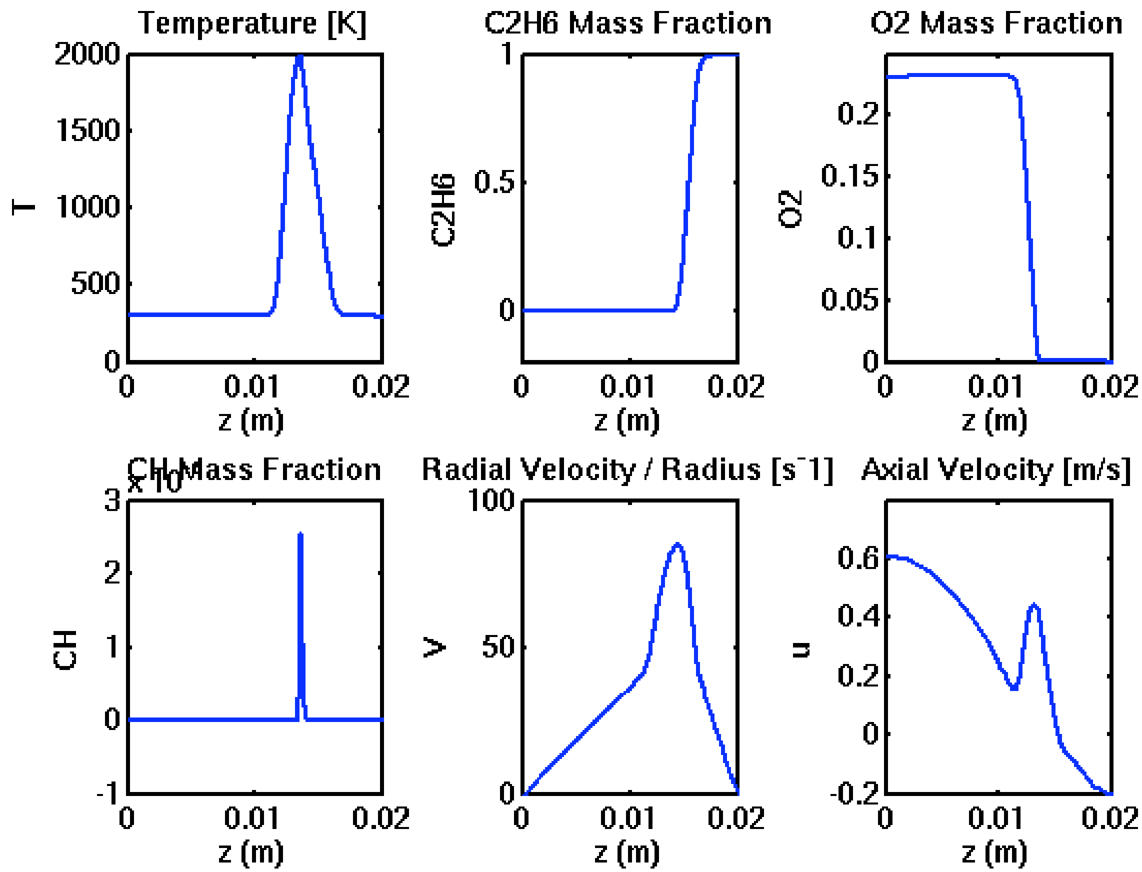
And Some Features:

- MATLAB Toolbox
- Python Interface
- C++ kernel
- Fast algorithms
- Object-oriented
- Backward-compatible with Chemkin-II
- Run under Windows, linux, Mac OS X, unix, ...
- open source

A few things Cantera can do...

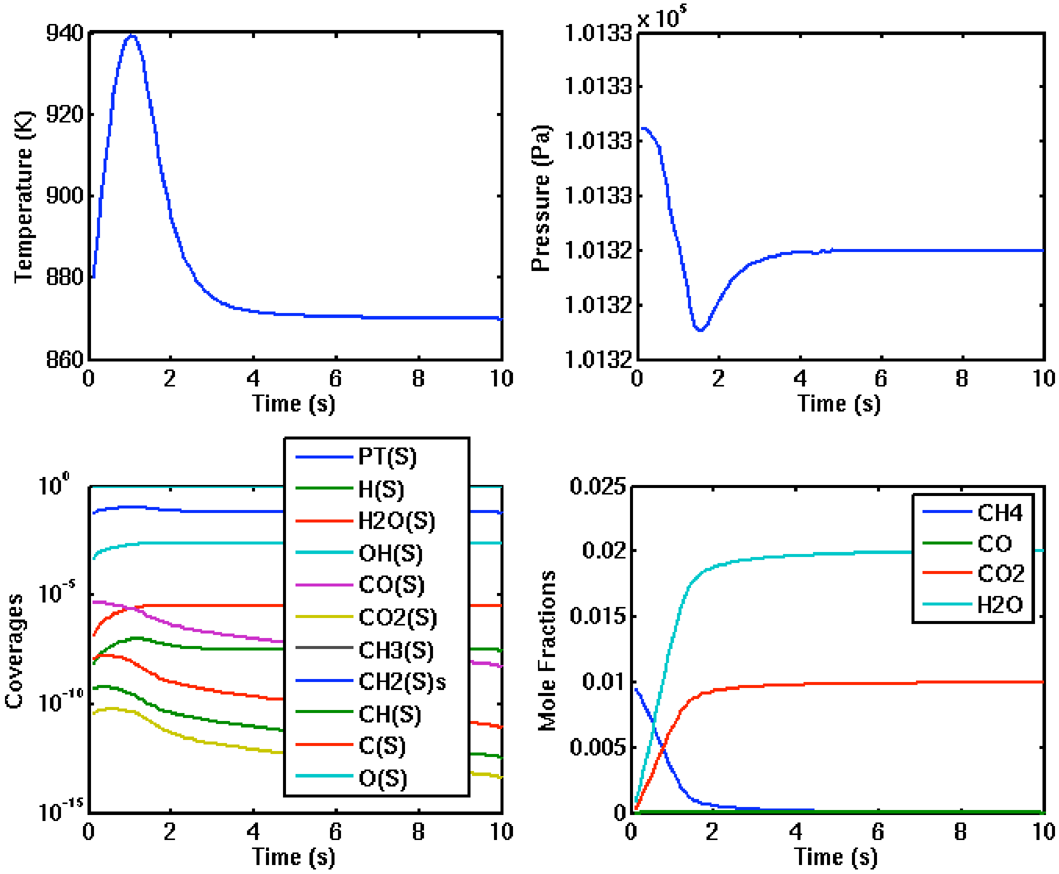
Counterflow Diffusion Flame

Non-premixed, ethane/air opposed-jet flame at 1 atm pressure



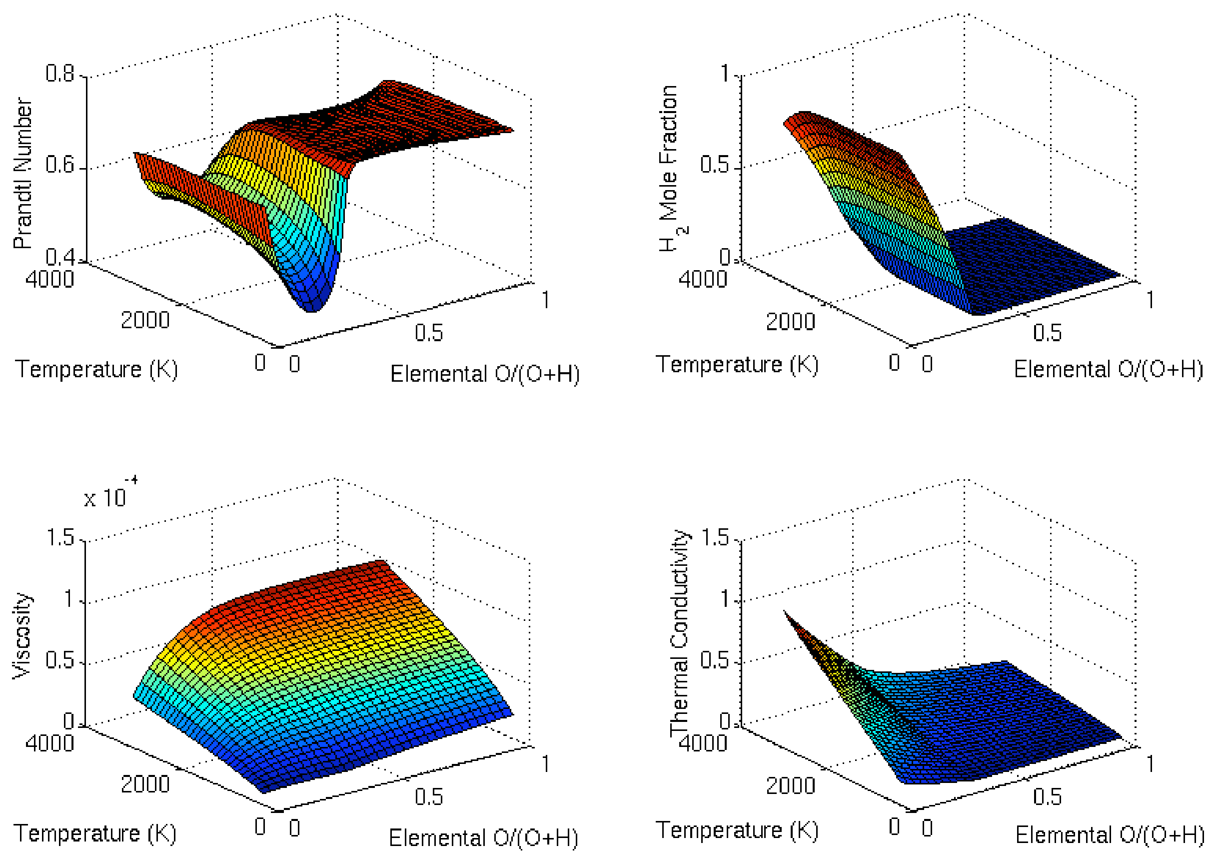
Heterogeneous chemistry

Oxidation of a1% methane in air mixture on a 1 cm^2 Pt foil.
Pt catalytic combustion mechanism is from Deutschman et al., Proc. 26th Symp. (Intl.) on Combustion,1996, pp. 1747-1754



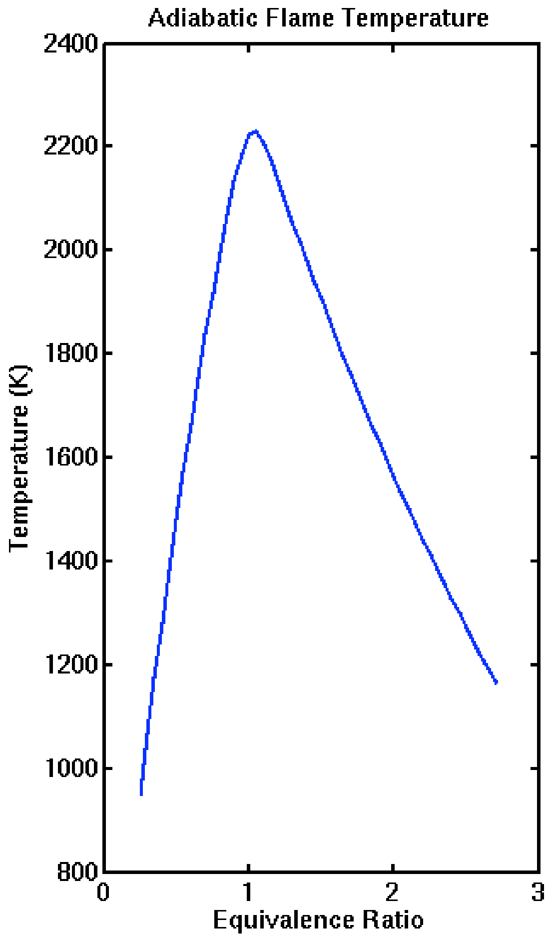
Transport Properties

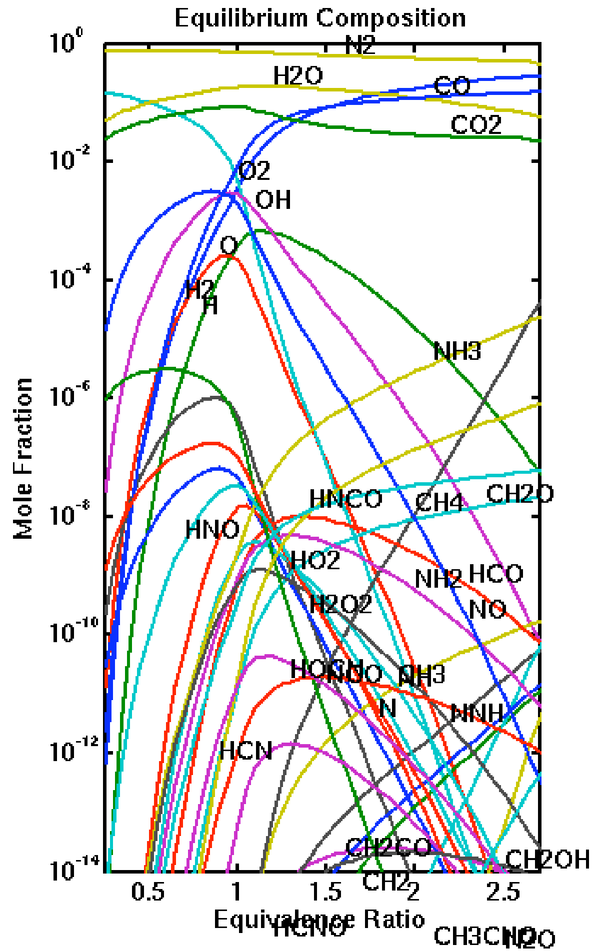
Prandtl number of an equilibrium H/O mixture



Chemical Equilibrium

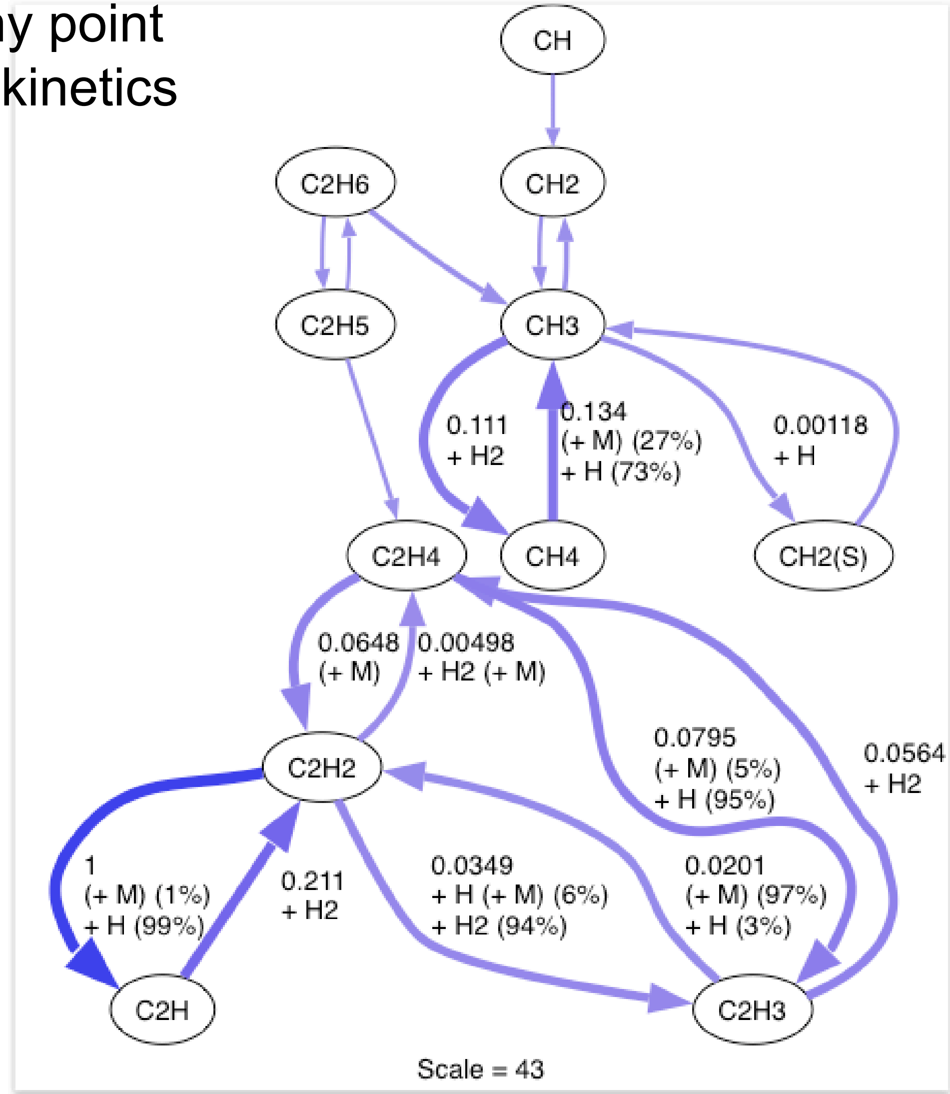
Adiabatic flame temperature for methane/air as a function of equivalence ratio





Reaction Path Diagrams

view chemical pathways at any point in a flame, or at any time in a kinetics simulation

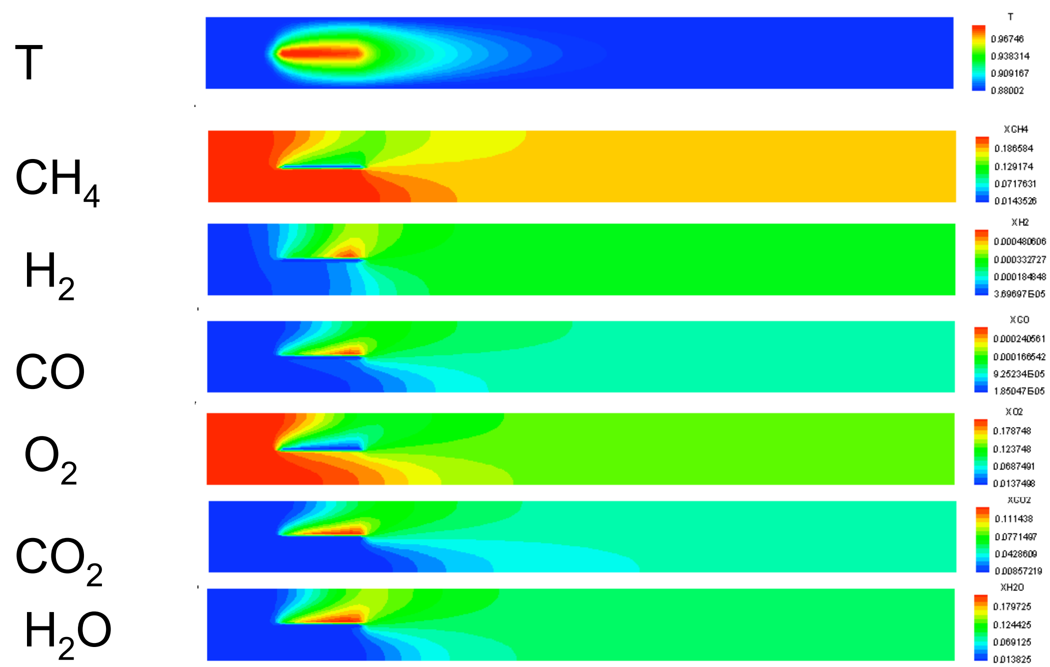


Cantera can be used from applications written in Fortran, C, C++, ...

- Use it to
  - evaluate thermodynamic and/or transport properties
  - compute chemical equilibrium
  - calculate homogeneous and heterogeneous reaction rates
  - evaluate liquid/vapor equilibria
  - ...
- Use it with commercial CFD packages (Fluent, ...)

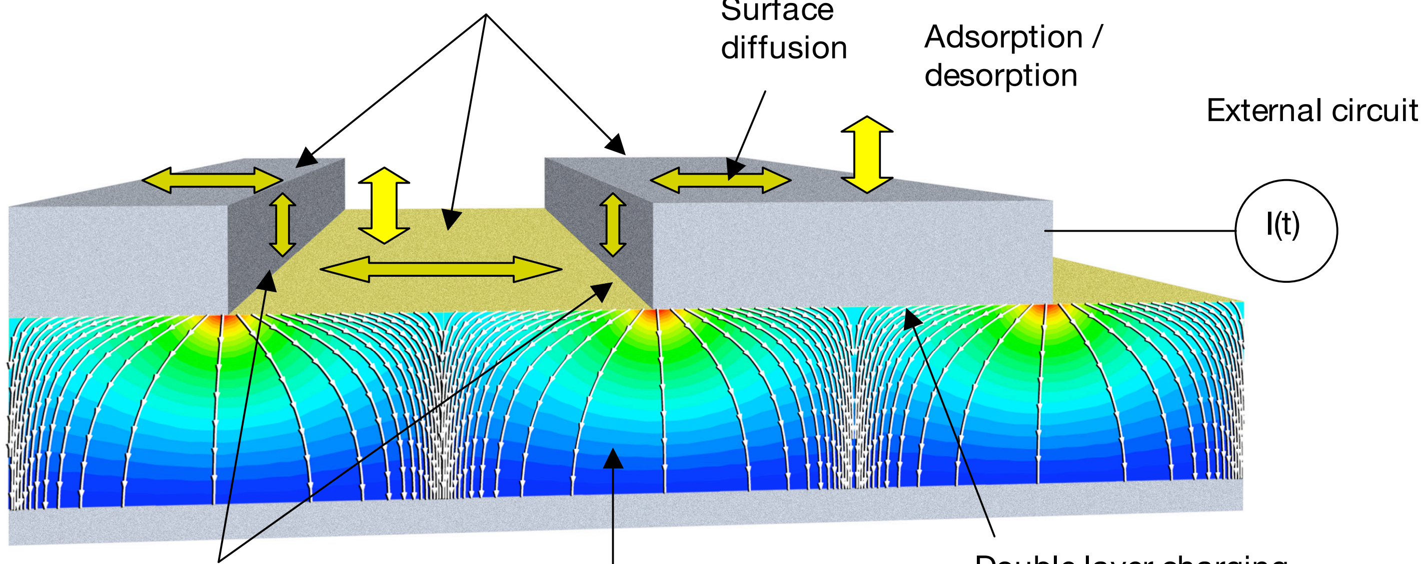
Example: a 2D model of a single-chamber fuel cell

- Fortran 90 main program
- Cantera used for
  - Transport properties
  - Heterogeneous reaction rates in porous electrodes
  - Multi-domain stiff solver



Another example: a transient model of SOFC "pattern anode" experiments

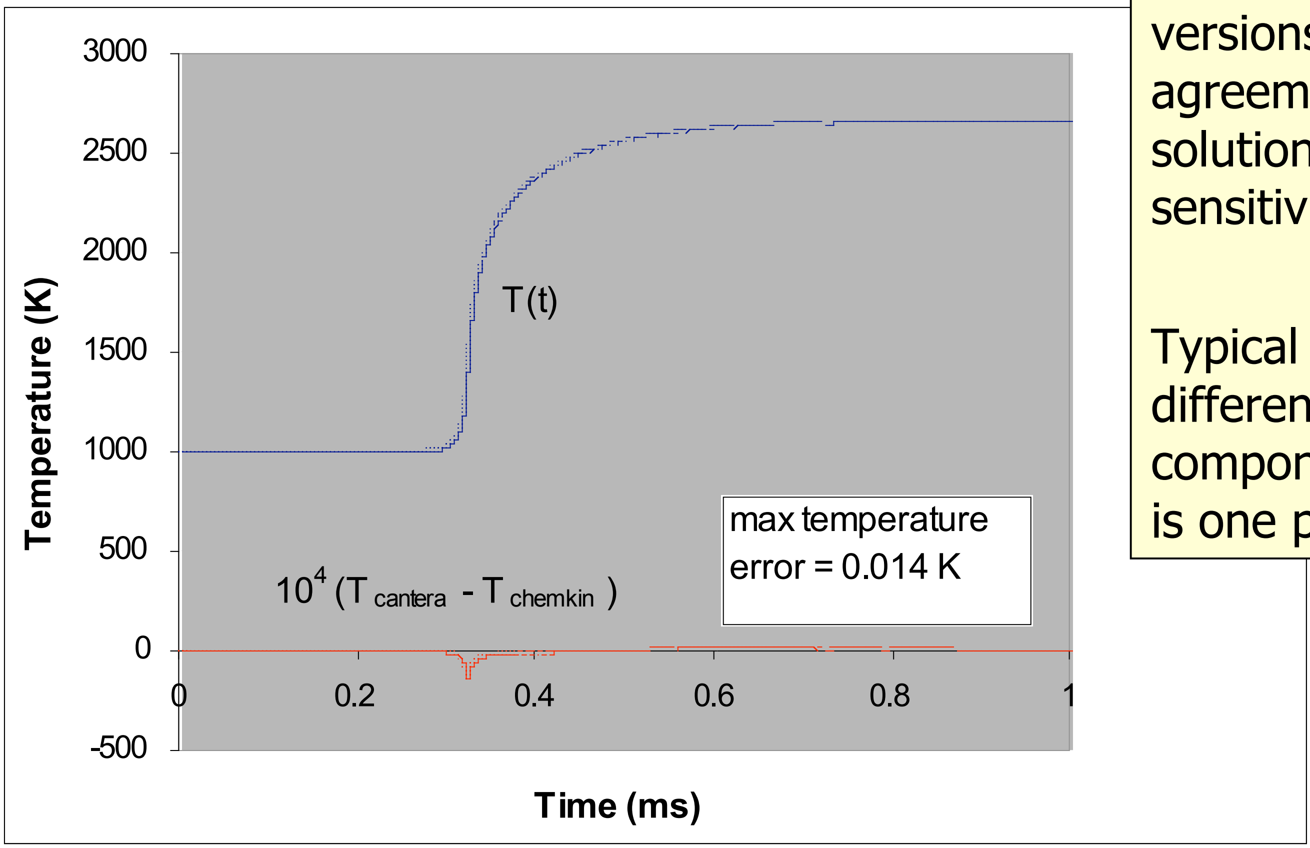
- C++ application
- Cantera used for
  - thermodynamic properties
  - heterogeneous reaction rates on two 2D surface phases and at the 1D "triple-phase boundary"



Validation and Benchmarks

Benchmark Validation

SENKIN / Chemkin-II vs. SENKIN / Cantera



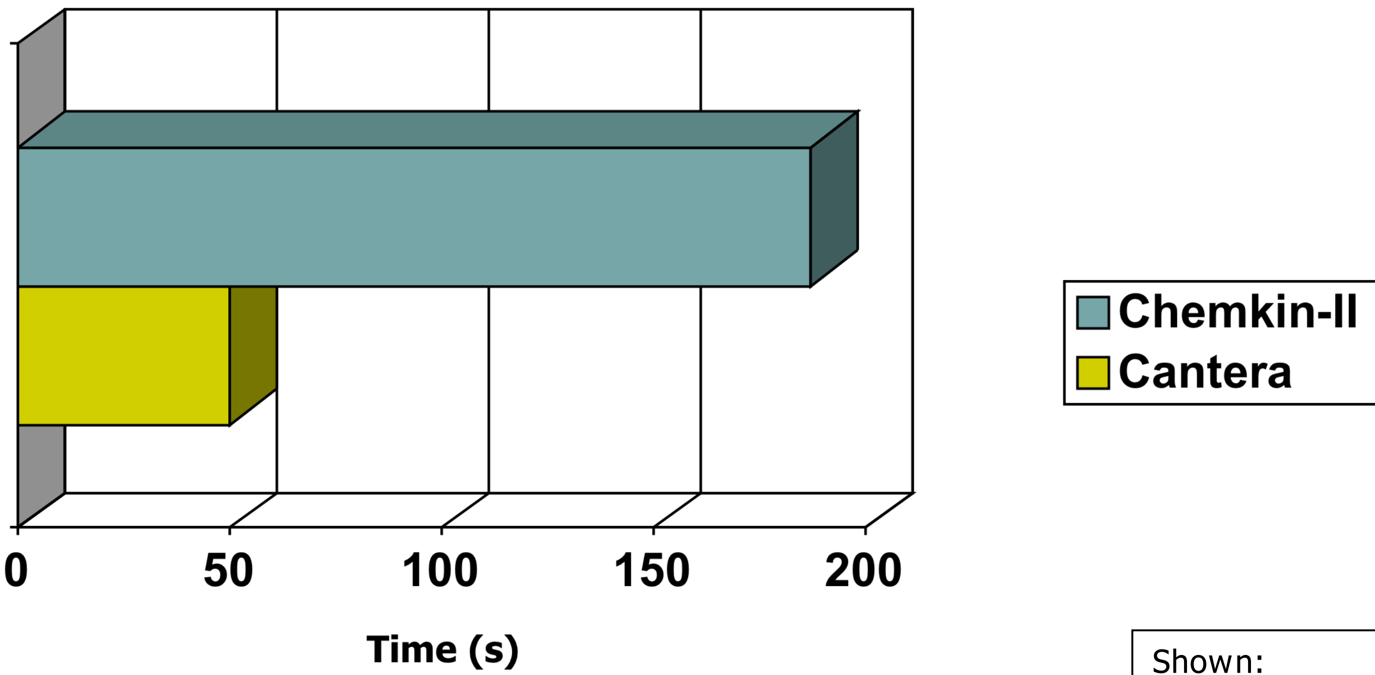
Cantera and Chemkin-II versions are in excellent agreement for all solution variables and sensitivity coefficients.

Typical relative difference in any component at any time is one part in 10^6 or 10^7

Benchmark Performance

Constant P, H Problem with Sensitivity Analysis

Cantera is significantly faster for this benchmark on all platforms tested
(Linux, Windows, OSF/1, IRIX)

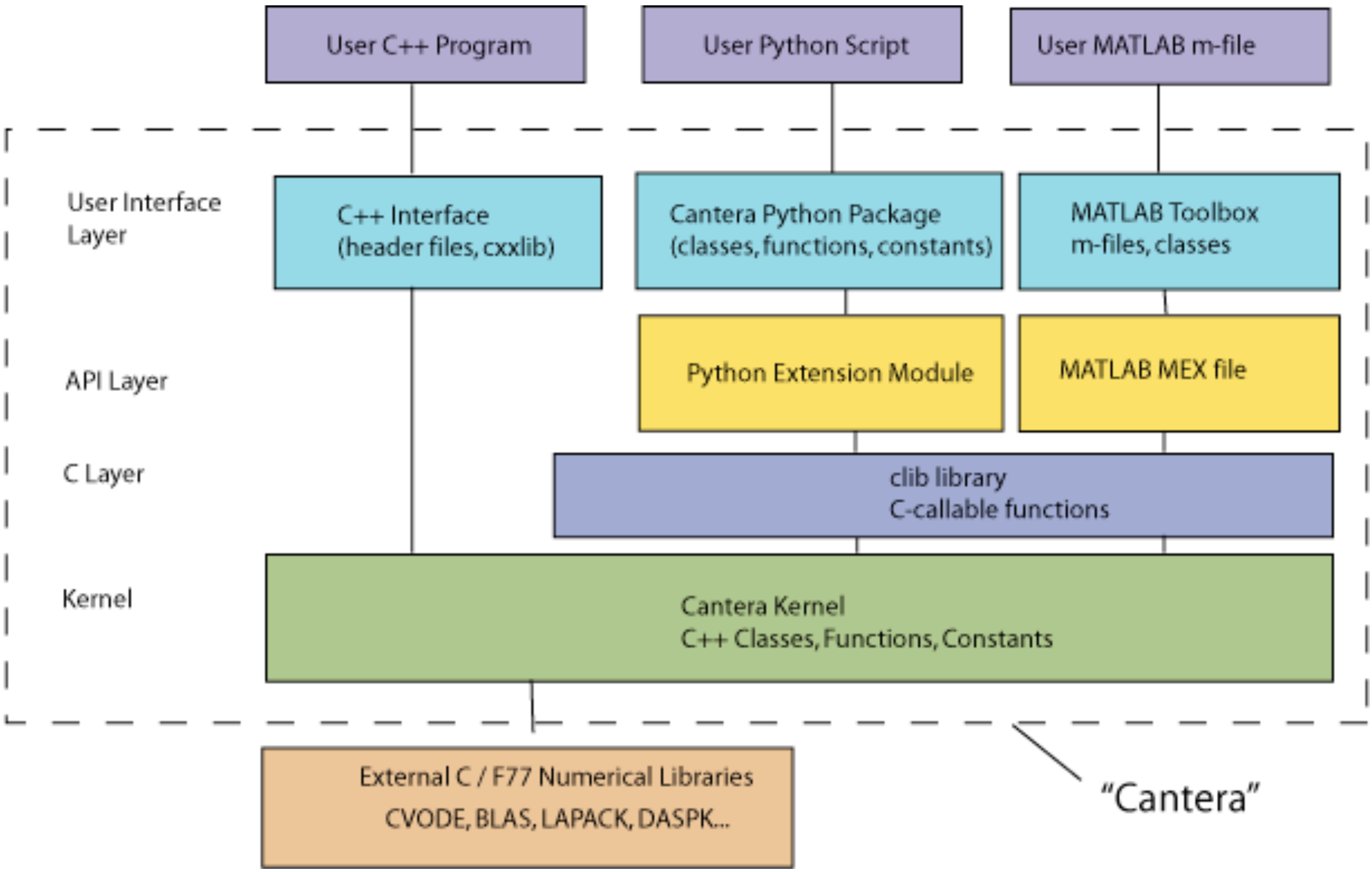


Shown:
Compaq Visual Fortran
MS Visual C++
750 MHz Pii

Note: these tests were conducted with an earlier version of Cantera.

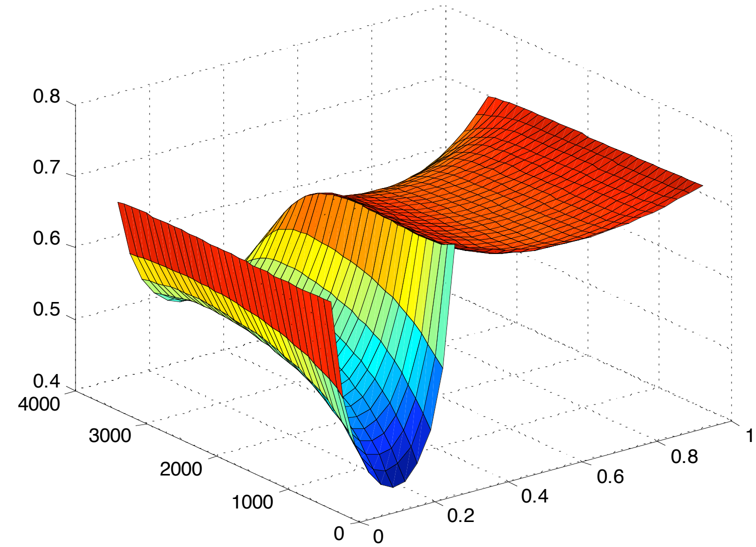
Cantera Structure

Cantera Structure



The Cantera MATLAB Toolbox

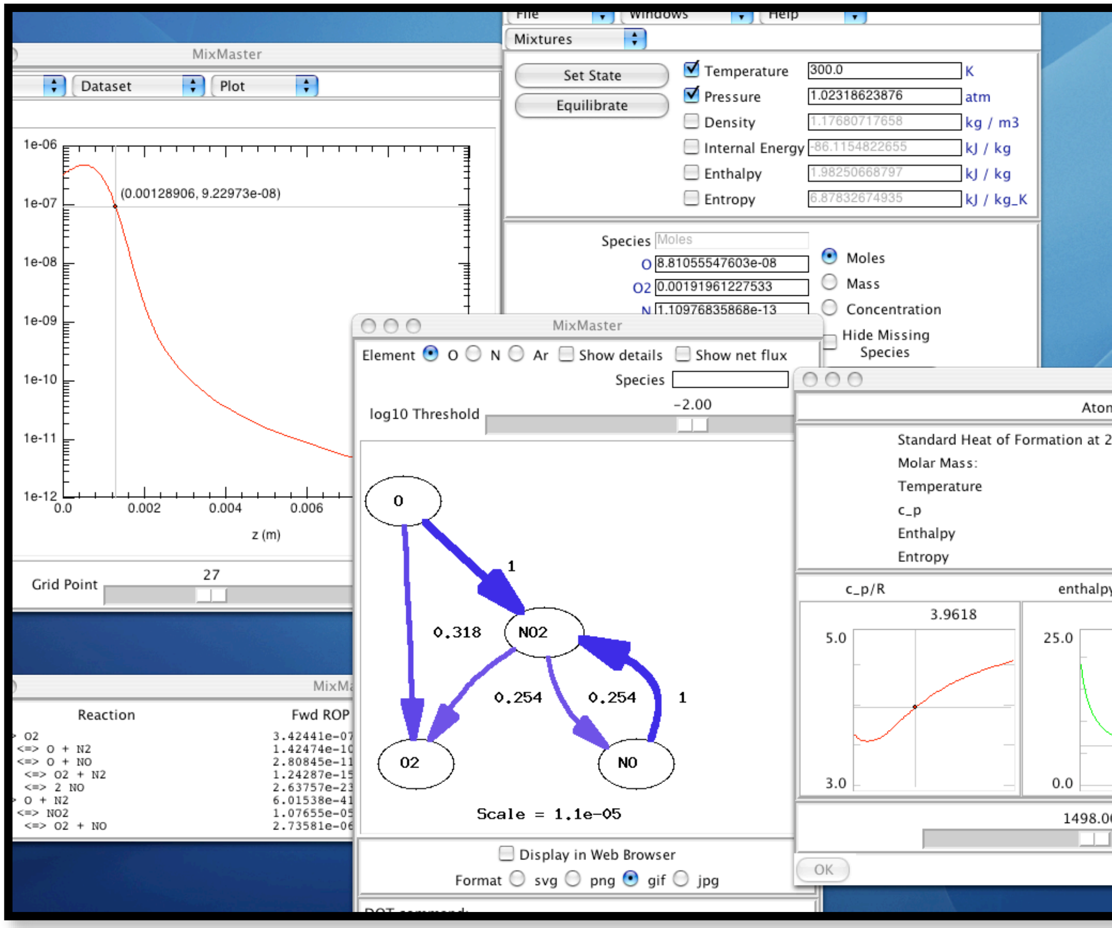
- MATLAB is a widely-used technical problem solving environment
- Excellent capabilities for numerical mathematics
  - Linear algebra
  - ODEs, PDEs
- Toolboxes implement application-specific capabilities
- The Cantera toolbox brings kinetics, thermo, and transport functionality to MATLAB



Example: Prandtl number for an equilibrium O/H mixture, computed using multicomponent transport properties

The Cantera Python Interface

- Python is an easy-to-use object-oriented scripting language
- Easy to create graphical applications
- Python comes preinstalled on most linux and Mac machines; a version for Windows is also available
- Used in several large-scale scientific computing projects for top-level user environment



Screen shot of MixMaster, a Cantera application written in Python

Cantera has a similar ‘look and feel’ in all environments

MATLAB

```
gas = GRI30;
set(gas,'T',300.0,'P',OneAtm,'X','CH4:1,O2:2,N2:7.52');
equilibrate(gas,'HP');
disp(gas)
```

Python

```
from Cantera import *
gas = GRI30()
gas.set(T = 300.0, P = OneAtm, X = 'CH4:1,O2:2,N2:7.52')
gas.equilibrate('HP')
print gas
```

C++

```
#include "Cantera.h"
#include "GRI30.h"
#include "equilibrium.h"

main() {
    GRI30 gas;
    gas.setState_TPX(300.0, OneAtm, "CH4:1,O2:2,N2:7.52");
    equilibrate(gas, "HP");
    cout << gas;
}
```

All three of these programs carry out the same calculation, with the same results

temperature	2225.52	K
pressure	101325	Pa
density	0.150193	kg/m^3
mean mol. weight	27.4283	amu

	1 kg	1 kmol	
enthalpy	-254590	-6.983e+06	J
internal energy	-929223	-2.549e+07	J
entropy	9876.57	2.709e+05	J/K
Gibbs function	-2.22351e+07	-6.099e+08	J
heat capacity c_p	1514.35	4.154e+04	J/K
heat capacity c_v	1211.21	3.322e+04	J/K

	X	Y
H2	3.604526e-03	2.649191e-04
H	3.903469e-04	1.434452e-05
O	2.156588e-04	1.257973e-04
O2	4.622237e-03	5.392454e-03
OH	2.875407e-03	1.782938e-03
H2O	1.834666e-01	1.205032e-01
HO2	4.989233e-07	6.003949e-07
H2O2	4.573249e-08	5.671420e-08
C	2.217810e-17	9.711895e-18
CH	3.361535e-18	1.595562e-18
CH2	9.827346e-18	5.025715e-18
CH2(S)	5.956345e-19	3.046081e-19
CH3	6.223564e-17	3.411442e-17
CH4	3.032972e-17	1.773977e-17
CO	8.987939e-03	9.178675e-03
CO2	8.536422e-02	1.369701e-01
HCO	7.949764e-10	8.410608e-10
CH2O	1.319499e-11	1.444479e-11
CH2OH	4.114099e-17	4.654961e-17
CH3O	6.575072e-19	7.439468e-19
CH3OH	3.492911e-18	4.080466e-18
C2H	3.671127e-24	3.350115e-24
C2H2	9.146744e-22	8.683058e-22
C2H3	6.921523e-27	6.824995e-27
C2H4	7.230037e-27	7.394897e-27
C2H5	7.843632e-32	8.310722e-32
C2H6	5.697162e-33	6.245789e-33
HCCO	5.366464e-20	8.027556e-20
CH2CO	7.105980e-20	1.089078e-19
HCCOH	6.968486e-23	1.068006e-22
N	1.424539e-08	7.274647e-09
NH	2.359734e-09	1.291754e-09
NH2	9.409152e-10	5.496479e-10
NH3	2.686508e-09	1.668083e-09
NNH	7.555846e-10	7.994703e-10
NO	1.888206e-03	2.065666e-03
NO2	3.462822e-07	5.808190e-07
N2O	1.001874e-07	1.607657e-07
HNO	3.366350e-08	3.806438e-08
CN	6.774013e-14	6.425636e-14
HCN	1.930651e-11	1.902309e-11
H2CN	5.477443e-18	5.598318e-18
HCNN	1.316652e-21	1.969694e-21
HCNO	1.020209e-16	1.600336e-16
HOCN	1.131156e-12	1.774372e-12
HNCO	3.864622e-10	6.062186e-10
NCO	1.543840e-11	2.364990e-11
N2	7.085838e-01	7.237005e-01
AR	0.000000e+00	0.000000e+00
C3H7	3.540964e-47	5.562683e-47
C3H8	2.428377e-48	3.904100e-48
CH2CHO	2.952869e-25	4.634145e-25
CH3CHO	5.854760e-26	9.403438e-26

The Cantera Kernel

- C++ class libraries
- Designed for performance
  - Property caching
  - Virtual methods used sparingly
  - Low-level methods written to maximize inlining
  - CPU-intensive code hand-optimized
- Uses standard open-source numerical libraries
  - BLAS, LAPACK, CVODE, DASPK

What's on the CD?

- Documentation
  - HTML pages documenting
    - The Cantera Python Package
    - The C++ kernel
  - Documents and presentations describing input files, F77 interfacing, installation procedures, etc.
  - Some workshop materials
- Source Code
  - The latest version of the full source distribution
- Third-party applications
  - Python 2.3.4, Numeric, and graphviz installers (Win/Mac)
- Binary installers for Windows and Mac platforms
  - MATLAB toolbox
  - Python Package
  - libraries and header files for building C++ or Fortran applications