PECOS

Predictive Engineering and Computational Sciences

Fully-Implicit Navier-Stokes (FIN-S)

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Acknowledgments

PECOS Collaborators & Support

- Todd Oliver
- Roy Stogner
- Marco Panesi
- Karl Schulz
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- Graham Carey
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- Brandon Oliver
- Jay LeBeau
- Randy Lillard

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- Ryan Bond

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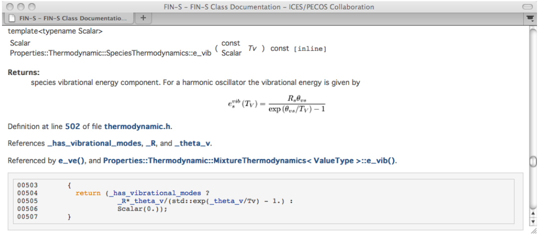
- Michael Wright
- Todd White
- Joe Olejniczak

- FIN-S is a SUPG finite element code for flow problems under active development at NASA Lyndon B. Johnson Space Center and within PECOS
  - The code is built on top of the `libMesh` parallel, adaptive finite element library
  - The initial implementation of the code targeted supersonic/hypersonic laminar calorically perfect gas flows & conjugate heat transfer
  - Initial extension to thermochemical nonequilibrium about 9 months ago
  - The technologies in FIN-S have been enhanced through a strongly collaborative research effort with Sandia National Labs
- NASA has allowed me to work here with the PECOS team since September
- FIN-S background and high-level overview was first presented to the DOE review team in October
- This talk will highlight some of new capabilities and discuss ongoing efforts

Development Environment

- Integration into PECOS Redmine development environment
  - Source tree now housed under PECOS `svn` repository
  - Redmine ticket system is being used to track feature requests, bugfixes, etc. . .
  - Automatic Buildbot regression testing
- Doxygen-based source code documentation
- Rigorous modeling document
- Example suite, unit tests, regression tests
- GNU `automake` build system



FIN-S Code Reuse and Dependencies

- `autoconf`
- `automake`
- `libtool`
- Boost
- Cantera
- `libMesh`

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Governing Equations

- Extension from a single-species calorically perfect gas to a reacting mixture of thermally perfect gases requires species conservation equations and additional energy transport mechanisms

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \ \boldsymbol{u}) \ = 0$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u} \boldsymbol{u}) = -\boldsymbol{\nabla} P + \boldsymbol{\nabla} \cdot \boldsymbol{\tau}$$

$$\frac{\partial \rho E}{\partial t} + \boldsymbol{\nabla} \cdot (\rho H \boldsymbol{u}) = -\boldsymbol{\nabla} \cdot \dot{\boldsymbol{q}} + \boldsymbol{\nabla} \cdot (\boldsymbol{\tau} \boldsymbol{u})$$

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$$
\begin{aligned}
\frac{\partial \rho_s}{\partial t} + \boldsymbol{\nabla} \cdot (\rho_s \boldsymbol{u}) &= \boldsymbol{\nabla} \cdot (\rho \mathcal{D}_s \boldsymbol{\nabla} c_s) + \dot{\omega}_s \\
\frac{\partial \rho \boldsymbol{u}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}\boldsymbol{u}) &= -\boldsymbol{\nabla} P + \boldsymbol{\nabla} \cdot \boldsymbol{\tau} \\
\frac{\partial \rho E}{\partial t} + \boldsymbol{\nabla} \cdot (\rho H \boldsymbol{u}) &= -\boldsymbol{\nabla} \cdot \dot{\boldsymbol{q}} + \boldsymbol{\nabla} \cdot (\boldsymbol{\tau} \boldsymbol{u}) + \boldsymbol{\nabla} \cdot \left(\rho \sum_{s=1}^{ns} h_s \mathcal{D}_s \boldsymbol{\nabla} c_s \right)
\end{aligned}
$$

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\end{aligned}
$$

- Problem class may also require a multitemperature thermal nonequilibrium option

$$
\frac{\partial \rho e_V}{\partial t} + \boldsymbol{\nabla} \cdot (\rho e_V \boldsymbol{u}) = -\boldsymbol{\nabla} \cdot \dot{\boldsymbol{q}}_V + \boldsymbol{\nabla} \cdot \left(\rho \sum_{s=1}^{ns} e_{V s} \mathcal{D}_s \boldsymbol{\nabla} c_s \right) + \dot{\omega}_V
$$

Thermodynamics & Transport Properties

- Thermochemistry models have been extended for a mixture of vibrationally and electronically excited thermally perfect gases

$$\begin{aligned} e^{\text{int}} =& e^{\text{trans}} + e^{\text{rot}} + e^{\text{vib}} + e^{\text{elec}} + h^0 \\ =& \sum_{s=1}^{ns} c_s e_s^{\text{trans}}(T) + \sum_{s=mol} c_s e_s^{\text{rot}}(T) + \\ & \sum_{s=mol} c_s e_s^{\text{vib}}(T_V) + \sum_{s=1}^{ns} c_s e_s^{\text{elec}}(T_V) + \sum_{s=1}^{ns} c_s h_s^0 \end{aligned}$$

  Here we have assumed that $T^{\text{trans}} = T^{\text{rot}} = T$ and $T^{\text{vib}} = T^{\text{elec}} = T_V$

- The transport properties have been extended as required
  - Species viscosity given by Blottner curve fits
  - Species conductivities determined from an Eucken relation
  - Mixture transport properties computed via Wilke's mixing rule
  - Mass diffusion currently treated by assuming constant Lewis number

Chemical Kinetics

- We consider r general reactions of the form

$$\mathsf{N}_2 + \mathcal{M} \rightleftharpoons 2\mathsf{N} + \mathcal{M}$$
$$\cdots$$
$$\mathsf{N}_2 + \mathsf{O} \rightleftharpoons \mathsf{NO} + \mathsf{N}$$
$$\cdots$$

- The reactions are of the form

$$\mathcal{R}_r = k_{br} \prod_{s=1}^{ns} \left(\frac{\rho_s}{M_s} \right)^{\beta_{sr}} - k_{fr} \prod_{s=1}^{ns} \left(\frac{\rho_s}{M_s} \right)^{\alpha_{sr}}$$

where α_{sr} and β_{sr} are the stoichiometric coefficients for reactants and products

- The source terms are then

$$\dot{\omega}_s = M_s \sum_{r=1}^{nr} (\alpha_{sr} - \beta_{sr}) (\mathcal{R}_{br} - \mathcal{R}_{fr})$$

Kinetic Rates

- The forward rate coefficients are defined with a modified Arrhenius law as a function of some temperature $\bar{T}$

$$k_{fr}\left(\bar{T}\right) = C_{fr}\bar{T}^{\eta_r}\exp\left(-E_{ar}/R\bar{T}\right)$$

  where the rate constants are determined empirically.
- The corresponding backward rate coefficient can be found using the principle of detailed balance and the equilibrium constant K_{eq}

$$K_{eq} = \frac{k_{fr}}{k_{br}}$$

- In thermal equilibrium $\bar{T} = T$. We are currently using CANTERA in this regime.
- In thermal nonequilibrium $\bar{T} = \bar{T}\left(T, T_V\right)$ and typical hackery ensues.

Turbulence Models

- Use standard closure assumptions and eddy viscosity models
- Spalart-Allmaras: $\mu_t = \bar{\rho}\nu_{sa} f_{v1}$

$$\frac{\partial \bar{\rho}\nu_{sa}}{\partial t} + \boldsymbol{\nabla} \cdot (\bar{\rho}\tilde{\boldsymbol{u}}\nu_{sa}) = c_{b1} S_{\mathrm{sa}} \bar{\rho}\nu_{sa} - c_{w1} f_w \bar{\rho} \left(\frac{\nu_{sa}}{d}\right)^2 + \frac{1}{\sigma}\boldsymbol{\nabla} \cdot [(\bar{\mu} + \bar{\rho}\nu_{sa})\boldsymbol{\nabla}\nu_{sa}] + \frac{c_{b2}}{\sigma}\bar{\rho}\boldsymbol{\nabla}\nu_{sa} \cdot \boldsymbol{\nabla}\nu_{sa}$$

- k–ω (1988): $\mu_t = \bar{\rho}k/\omega$

$$\frac{\partial \bar{\rho}k}{\partial t} + \boldsymbol{\nabla} \cdot (\bar{\rho}\tilde{\boldsymbol{u}}k) = \boldsymbol{\tau} : \boldsymbol{\nabla}\tilde{\boldsymbol{u}} - \beta^* \bar{\rho}k\omega + \boldsymbol{\nabla} \cdot [(\bar{\mu} + \sigma^* \mu_t)\, \boldsymbol{\nabla} k]$$

$$\frac{\partial \bar{\rho}\omega}{\partial t} + \boldsymbol{\nabla} \cdot (\bar{\rho}\tilde{\boldsymbol{u}}\omega) = \alpha\frac{\omega}{k}\boldsymbol{\tau} : \boldsymbol{\nabla}\tilde{\boldsymbol{u}} - \beta\bar{\rho}\omega^2 + \boldsymbol{\nabla} \cdot [(\bar{\mu} + \sigma\mu_t)\, \boldsymbol{\nabla}\omega]$$

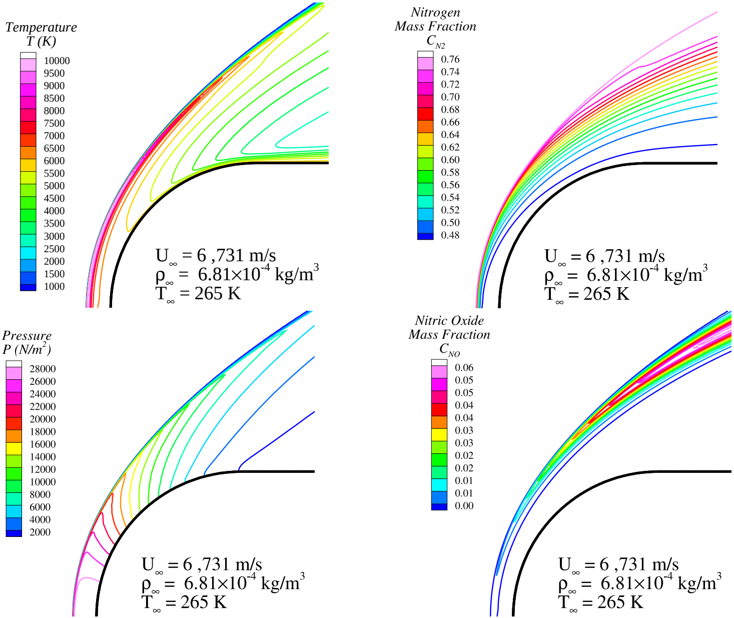
- k–ω (2006) and SST soon to come

2D Extended Cylinder

- Laminar flow in thermal equilibrium
- No-slip, adiabatic, noncatalytic wall
- Chemical nonequilibrium, 5 species air (78% N_2, 22% O_2)

$$
\begin{aligned}
U_\infty &= 6,731 \,{}^{\mathrm{m}}\!/\!{}_{\mathrm{sec}} \\
\rho_\infty &= 6.81 \times 10^{-4} \,{}^{\mathrm{kg}}\!/\!{}_{\mathrm{m}^3} \\
T_\infty &= 265\,\mathrm{K}
\end{aligned}
$$

- Blottner/Wilke/Eucken with constant Lewis number $Le = 1.4$ for transport properties
- Mesh, iterative convergence
- FIN-S/DPLR comparison
- Weak & Strong Scaling


Temperature
T (K)
10000
9500
9000
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
U∞ = 6 ,731 m/s
ρ∞ = 6.81×10^-4 kg/m^3
T∞ = 265 K
Nitrogen
Mass Fraction
C_N2
0.76
0.74
0.72
0.70
0.68
0.66
0.64
0.62
0.60
0.58
0.56
0.54
0.52
0.50
0.48
U∞ = 6 ,731 m/s
ρ∞ = 6.81×10^-4 kg/m^3
T∞ = 265 K
Pressure
P (N/m^2)
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
U∞ = 6 ,731 m/s
ρ∞ = 6.81×10^-4 kg/m^3
T∞ = 265 K
Nitric Oxide
Mass Fraction
C_NO
0.06
0.05
0.05
0.04
0.04
0.03
0.03
0.02
0.02
0.01
0.01
0.00
U∞ = 6 ,731 m/s
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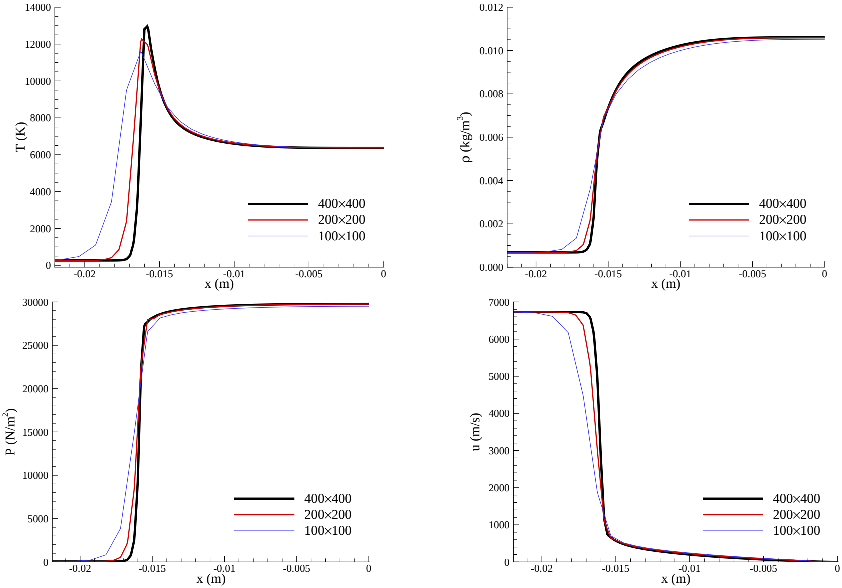
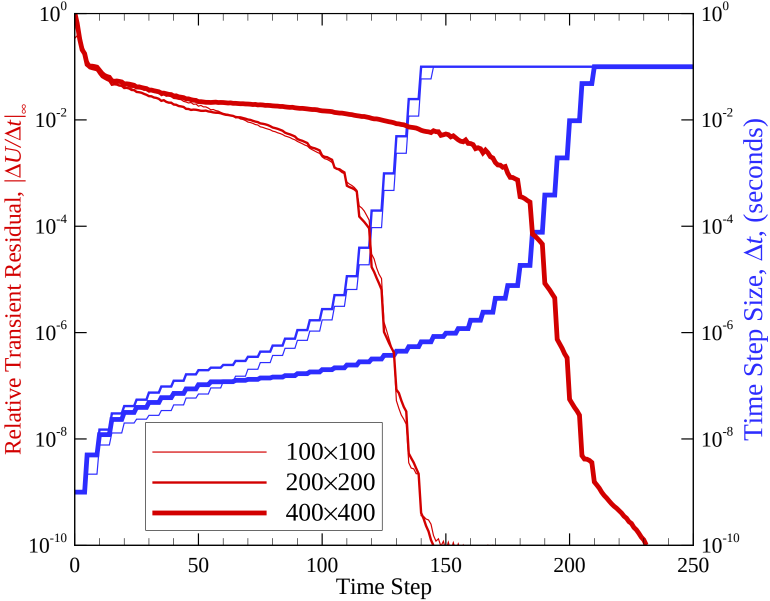
T∞ = 265 K

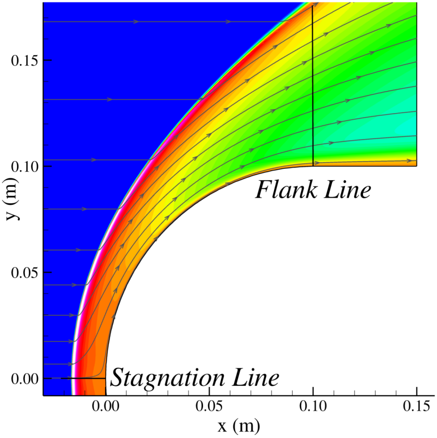
Mesh Convergence

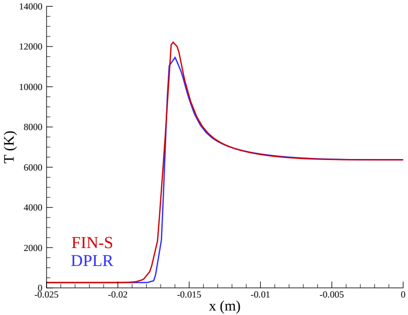


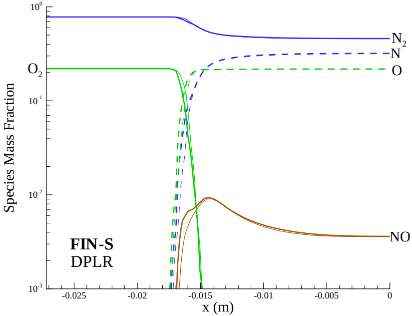
Iterative Convergence



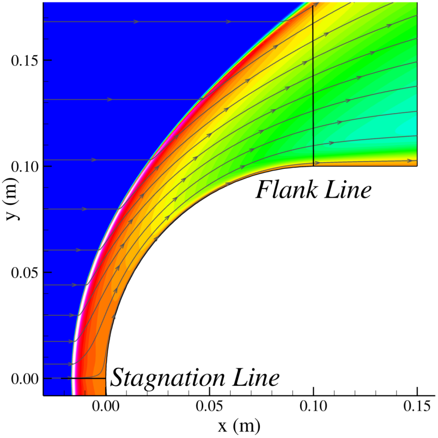
Code-to-Code Comparison – Stagnation Line

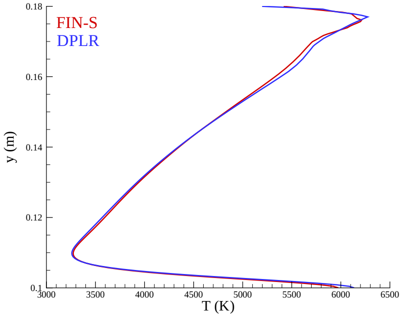


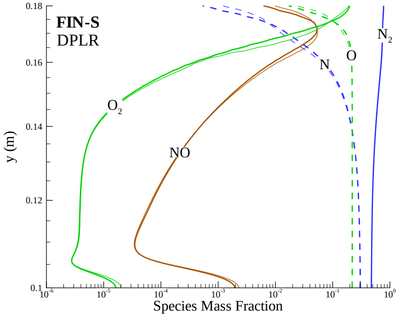




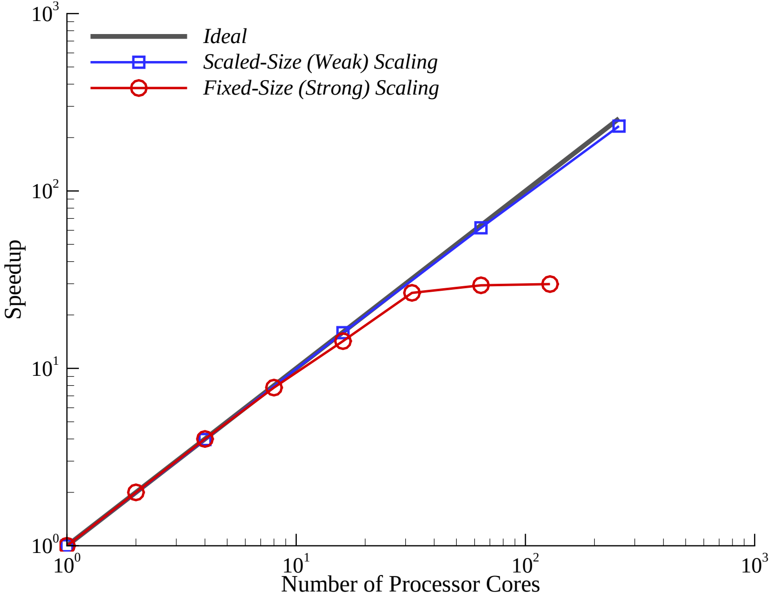
Code-to-Code Comparison –
Flank Line



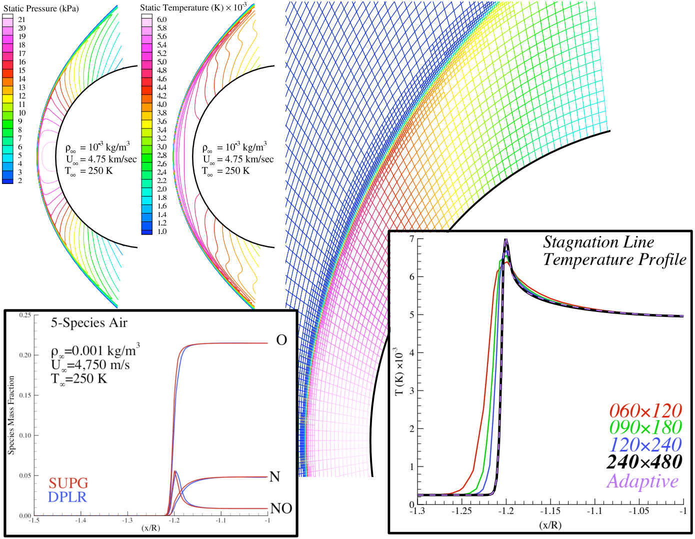




Speedup



Ideal
Scaled-Size (Weak) Scaling
Fixed-Size (Strong) Scaling
Speedup
Number of Processor Cores
10^0
10^1
10^2
10^3

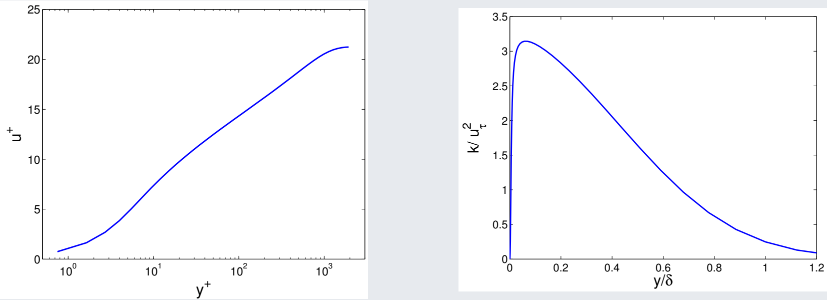


AMR – 13,079 node mesh, “spot on” with uniform 115,921 node mesh

Initial Turbulent Results

- Fully turbulent flow over a flat plate
- k-ω turbulence model; calorically perfect N_2; adiabatic wall
- $Re_L \approx 1 \times 10^6$; $M_\infty \approx 0.2$

Boundary layer profiles at trailing edge



Code and solution verification activities are ongoing

HTChem

- The high-temperature thermodynamic and transport models currently implemented in FIN-S are one of several possible choices, and serve to provide the minimum set required for algorithm development
- It is expected that these simplified models will be invalidated for certain problem classes and that more complex models will be required
- Similar thermochemical models are required by other areas of PECOS research, e.g. ablation and shock layer radiation
- The HTChem library is being developed to consolidate efforts and provide a common source for requisite high-temperature thermochemistry and transport property data

Manufactured Analytical Solution Abstraction Library

- Dearth of exact solutions necessitates *method of manufactured solutions*
- Some manufactured solutions exist for the calorically perfect Navier-Stokes equations
  - Developed in large part by Sandia National Labs
  - Specific solutions for field, boundary condition order-of-accuracy verification
- Existing solutions provide a necessary but not sufficient test suite
  - Will need to develop many more solutions to verify reacting flows with complex transport models
- Manufactured solutions are a valuable resource that should be accessible to anyone
- PECOS is developing the Manufactured Analytical Solution Abstraction (MASA) library to provide well-defined manufactured solutions and source terms for a range of physics applications

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Manufactured solutions are being constructed and will be incorporated into the FIN-S regression test suite

Manufactured analytical solutions (used by Roy, Smith, and Ober) for each one of the primitive variables in Navier-Stokes equations are:

$$
\begin{aligned}
\rho\left(x,y\right) &= \rho_0 + \rho_x \sin\left(\frac{a_{\rho x}\pi x}{L}\right) + \rho_y \cos\left(\frac{a_{\rho y}\pi y}{L}\right),\\
u\left(x,y\right) &= u_0 + u_x \sin\left(\frac{a_{ux}\pi x}{L}\right) + u_y \cos\left(\frac{a_{uy}\pi y}{L}\right),\\
v\left(x,y\right) &= v_0 + v_x \cos\left(\frac{a_{vx}\pi x}{L}\right) + v_y \sin\left(\frac{a_{vy}\pi y}{L}\right),\\
p\left(x,y\right) &= p_0 + p_x \cos\left(\frac{a_{px}\pi x}{L}\right) + p_y \sin\left(\frac{a_{py}\pi y}{L}\right)
\end{aligned}
$$

The method of manufactured solutions applied to Navier-Stokes equations requires modifying the governing equations by adding a source term to the right-hand side of each equation:

$$\frac{\partial(\rho)}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = Q_\rho$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p - \tau_{xx})}{\partial x} + \frac{\partial(\rho uv - \tau_{xy})}{\partial y} = Q_u$$

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho vu - \tau_{yx})}{\partial x} + \frac{\partial(\rho v^2 + p - \tau_{yy})}{\partial y} = Q_v$$

$$\frac{\partial(\rho e_t)}{\partial t} + \frac{\partial(\rho u e_t + pu - u\tau_{xx} - v\tau_{xy} + q_x)}{\partial x} + \frac{\partial(\rho v e_t + pv - u\tau_{yx} - v\tau_{yy} + q_y)}{\partial y} = Q_{e_t}$$

so the modified set of equations has a known, analytical solution.

Symbolic representations of requisite source terms and C-source code have recently been generated for 2D and 3D calorically perfect gas flows.

$$
\begin{aligned}
Q_\rho = {} & \frac{a_{\rho x}\pi\rho_x}{L}\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] \\
& -\frac{a_{\rho y}\pi\rho_y}{L}\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] \\
& +\frac{a_{ux}\pi u_x}{L}\cos\left(\frac{a_{ux}\pi x}{L}\right)\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
& +\frac{a_{vy}\pi v_y}{L}\cos\left(\frac{a_{vy}\pi y}{L}\right)\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]
\end{aligned}
$$

$$
\begin{aligned}
Q_u - {} & \frac{a_{px}\pi p_x}{L}\sin\left(\frac{a_{px}\pi x}{L}\right) \\
& +\frac{a_{\rho x}\pi\rho_x}{L}\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]^2 \\
& -\frac{a_{\rho y}\pi\rho_y}{L}\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] \\
& +\frac{2a_{ux}\pi u_x}{L}\cos\left(\frac{a_{ux}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
& -\frac{\pi a_{uy}u_y}{L}\sin\left(\frac{a_{uy}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
& +\frac{\pi a_{vy}v_y}{L}\cos\left(\frac{a_{vy}\pi y}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
& +\frac{4a_{ux}^2\pi^2\mu u_x}{3L^2}\sin\left(\frac{a_{ux}\pi x}{L}\right) \quad + \quad \frac{a_{uy}^2\pi^2\mu u_y}{L^2}\cos\left(\frac{a_{uy}\pi y}{L}\right)
\end{aligned}
$$

$$
\begin{aligned}
Q_v = {} & \frac{a_{py}\pi p_y}{L}\cos\left(\frac{a_{py}\pi y}{L}\right) \\
& +\frac{\pi a_{\rho x}\rho_x}{L}\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] \\
& -\frac{a_{\rho y}\pi\rho_y}{L}\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]^2 \\
& +\frac{a_{ux}\pi u_x}{L}\cos\left(\frac{a_{ux}\pi x}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
& -\frac{a_{vx}\pi v_x}{L}\sin\left(\frac{a_{vx}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
& +\frac{2a_{vy}\pi v_y}{L}\cos\left(\frac{a_{vy}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
& +\frac{a_{vx}^2\pi^2\mu v_x}{L^2}\cos\left(\frac{a_{vx}\pi x}{L}\right)+\frac{4a_{vy}^2\pi^2\mu v_y}{3L^2}\sin\left(\frac{a_{vy}\pi y}{L}\right)
\end{aligned}
$$

$$
\begin{aligned}
Q_{e_t} = {} & -\frac{a_{px}\pi p_x}{L}\frac{\gamma}{\gamma-1}\sin\left(\frac{a_{px}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] \\
& +\frac{a_{py}\pi p_y}{L}\frac{\gamma}{\gamma-1}\cos\left(\frac{a_{py}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] \\
& +\frac{a_{\rho x}\pi\rho_x}{2L}\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]^2+\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]^2\right] \\
& -\frac{a_{\rho y}\pi\rho_y}{2L}\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]^2+\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]^2\right] \\
& +\frac{a_{ux}\pi u_x}{2L}\cos\left(\frac{a_{ux}\pi x}{L}\right)\left\{\left[p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_0\right]\frac{2\gamma}{\gamma-1}+\right. \\
& \qquad \left.+\left[3\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]^2+\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]^2\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]\right\} \\
& -\frac{a_{uy}\pi u_y}{L}\sin\left(\frac{a_{uy}\pi y}{L}\right)\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] \\
& -\frac{a_{vx}\pi v_x}{L}\sin\left(\frac{a_{vx}\pi x}{L}\right)\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] \\
& +\frac{a_{vy}\pi v_y}{2L}\cos\left(\frac{a_{vy}\pi y}{L}\right)\left\{\left[p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_0\right]\frac{2\gamma}{\gamma-1}\right. \\
& \qquad \left.+\left[\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]^2+3\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]^2\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]\right\} \\
& +\frac{a_{px}^2\pi^2 k\,p_x\cos\left(\frac{a_{px}\pi x}{L}\right)}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]L^2R}+\frac{a_{py}^2\pi^2 k\,p_y\sin\left(\frac{a_{py}\pi y}{L}\right)}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]L^2R} \\
& -\frac{2a_{\rho x}^2\pi^2 k\,\rho_x^2}{L^2R}\cos^2\left(\frac{a_{\rho x}\pi x}{L}\right)\frac{\left[p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_0\right]}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^3} \quad - \quad \frac{a_{\rho x}^2\pi^2 k\rho_x}{L^2R}\sin\left(\frac{a_{\rho x}\pi x}{L}\right)\frac{\left[p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_0\right]}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^2} \\
& -\frac{2a_{\rho y}^2\pi^2 k\,\rho_y^2}{L^2R}\sin^2\left(\frac{a_{\rho y}\pi y}{L}\right)\frac{\left[p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_0\right]}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^3} \quad - \quad \frac{a_{\rho y}^2\pi^2 k\rho_y}{L^2R}\cos\left(\frac{a_{\rho y}\pi y}{L}\right)\frac{\left[p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_0\right]}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^2} \\
& +\frac{4a_{ux}^2\pi^2\mu u_x}{3L^2}\sin\left(\frac{a_{ux}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] \quad - \quad \frac{4a_{ux}^2\pi^2\mu u_x^2}{3L^2}\cos^2\left(\frac{a_{ux}\pi x}{L}\right) \\
& +\frac{a_{uy}^2\pi^2\mu u_y}{L^2}\cos\left(\frac{a_{uy}\pi y}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] \quad - \quad \frac{a_{uy}^2\pi^2\mu u_y^2}{L^2}\sin^2\left(\frac{a_{uy}\pi y}{L}\right) \\
& +\frac{a_{vx}^2\pi^2\mu v_x}{L^2}\cos\left(\frac{a_{vx}\pi x}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] \quad - \quad \frac{a_{vx}^2\pi^2\mu v_x^2}{L^2}\sin^2\left(\frac{a_{vx}\pi x}{L}\right) \\
& +\frac{4a_{vy}^2\pi^2\mu v_y}{3L^2}\sin\left(\frac{a_{vy}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] \quad - \quad \frac{4a_{vy}^2\pi^2\mu v_y^2}{3L^2}\cos^2\left(\frac{a_{vy}\pi y}{L}\right) \\
& -\frac{2a_{px}a_{\rho x}\pi^2 k\,p_x\rho_x}{L^2R}\frac{\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\sin\left(\frac{a_{px}\pi x}{L}\right)}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^2}-\frac{2a_{py}a_{\rho y}\pi^2 k\,p_y\rho_y}{L^2R}\frac{\cos\left(\frac{a_{py}\pi y}{L}\right)\sin\left(\frac{a_{\rho y}\pi y}{L}\right)}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^2} \\
& +\frac{4a_{ux}a_{vy}\pi^2\mu u_x v_y}{3L^2}\cos\left(\frac{a_{ux}\pi x}{L}\right)\cos\left(\frac{a_{vy}\pi y}{L}\right)-\frac{2a_{uy}a_{vx}\pi^2\mu u_y v_x}{L^2}\sin\left(\frac{a_{uy}\pi y}{L}\right)\sin\left(\frac{a_{vx}\pi x}{L}\right)
\end{aligned}
$$

NavierStokes_2d_e_code.C

```
#include <math.h>

double SourceQ_e ( double x, double y, double u_0, double u_x, double u_y,
                   double v_0, double v_x, double v_y,
                   double rho_0, double rho_x, double rho_y,
                   double p_0, double p_x, double p_y,
                   double a_px, double a_py,
                   double a_rhox, double a_rhoy,
                   double a_ux, double a_uy,
                   double a_vx, double a_vy,
                   double Gamma, double mu, double L)
{
  double Q_e;
  Q_e = -(v_x * cos(a_vx * PI * x / L) + v_y * sin(a_vy * PI * y / L) + v_0) * (pow(u_x * sin(a_ux * PI * x / L) + u_y * cos(a_uy * PI * y / L) + u_0, 0.2e1) + pow(v_x * cos(a_vx * PI * x / L) + v_y *
 sin(a_vy * PI * y / L) + v_0, 0.2e1)) * rho_y * sin(a_rhoy * PI * y / L) * a_rhoy * PI / L / 0.2e1 + (u_x * sin(a_ux * PI * x / L) + u_y * cos(a_uy * PI * y / L) + u_0) * (pow(u_x * sin(a_ux * PI * x
 / L) + u_y * cos(a_uy * PI * y / L) + u_0, 0.2e1) + pow(v_x * cos(a_vx * PI * x / L) + v_y * sin(a_vy * PI * y / L) + v_0, 0.2e1)) * rho_x * cos(a_rhox * PI * x / L) * a_rhox * PI / L / 0.2e1 + 0.4e1
 / 0.3e1 * (v_x * cos(a_vx * PI * x / L) + v_y * sin(a_vy * PI * y / L) + v_0) * mu * v_y * sin(a_vy * PI * y / L) * a_vy * a_vy * PI * PI * pow(L, -0.2e1) - 0.4e1 / 0.3e1 * mu * v_y * v_y * pow(cos(a
_vy * PI * y / L), 0.2e1) * a_vy * a_vy * PI * PI * pow(L, -0.2e1) - mu * v_x * v_x * pow(sin(a_vx * PI * x / L), 0.2e1) * a_vx * a_vx * PI * PI * pow(L, -0.2e1) - 0.4e1 / 0.3e1 * mu * u_x * u_x * pow
(cos(a_ux * PI * x / L), 0.2e1) * a_ux * a_ux * PI * PI * pow(L, -0.2e1) - mu * u_y * u_y * pow(sin(a_uy * PI * y / L), 0.2e1) * a_uy * a_uy * PI * PI * pow(L, -0.2e1) + (Gamma * (p_x * cos(a_px * PI 
* x / L) + p_y * sin(a_py * PI * y / L) + p_0) / (Gamma - 0.1e1) + (pow(u_x * sin(a_ux * PI * x / L) + u_y * cos(a_uy * PI * y / L) + u_0, 0.2e1) / 0.2e1 + 0.3e1 / 0.2e1 * pow(v_x * cos(a_vx * PI * x 
/ L) + v_y * sin(a_vy * PI * y / L) + v_0, 0.2e1)) * (rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rhoy * PI * y / L) + rho_0)) * v_y * cos(a_vy * PI * y / L) * a_vy * PI / L + (Gamma * (p_x * cos
(a_px * PI * x / L) + p_y * sin(a_py * PI * y / L) + p_0) / (Gamma - 0.1e1) + (0.3e1 / 0.2e1 * pow(u_x * sin(a_ux * PI * x / L) + u_y * cos(a_uy * PI * y / L) + u_0, 0.2e1) + pow(v_x * cos(a_vx * PI *
 x / L) + v_y * sin(a_vy * PI * y / L) + v_0, 0.2e1) / 0.2e1) * (rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rhoy * PI * y / L) + rho_0)) * u_x * cos(a_ux * PI * x / L) * a_ux * PI / L + (v_x * c
os(a_vx * PI * x / L) + v_y * sin(a_vy * PI * y / L) + v_0) * mu * v_x * cos(a_vx * PI * x / L) * a_vx * a_vx * PI * PI * pow(L, -0.2e1) + 0.4e1 / 0.3e1 * (u_x * sin(a_ux * PI * x / L) + u_y * cos(a_u
y * PI * y / L) + u_0) * mu * u_x * sin(a_ux * PI * x / L) * a_ux * a_ux * PI * PI * pow(L, -0.2e1) + (u_x * sin(a_ux * PI * x / L) + u_y * cos(a_uy * PI * y / L) + u_0) * mu * u_y * cos(a_uy * PI * y
 / L) * a_uy * a_uy * PI * PI * pow(L, -0.2e1) - (v_x * cos(a_vx * PI * x / L) + v_y * sin(a_vy * PI * y / L) + v_0) * (rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rhoy * PI * y / L) + rho_0) * (
u_x * sin(a_ux * PI * x / L) + u_y * cos(a_uy * PI * y / L) + u_0) * u_y * sin(a_uy * PI * y / L) * a_uy * PI / L - (p_x * cos(a_px * PI * x / L) + p_y * sin(a_py * PI * y / L) + p_0) * rho_x * k * si
n(a_rhox * PI * x / L) * a_rhox * a_rhox * PI * PI * pow(rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rhoy * PI * y / L) + rho_0, -0.2e1) * pow(L, -0.2e1) / R - (0.2e1 * p_x * cos(a_px * PI * x / 
L) + 0.2e1 * p_y * sin(a_py * PI * y / L) + 0.2e1 * p_0) * rho_x * rho_x * k * pow(cos(a_rhox * PI * x / L), 0.2e1) * a_rhox * a_rhox * PI * PI * pow(rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_r
hoy * PI * y / L) + rho_0, -0.3e1) * pow(L, -0.2e1) / R - (p_x * cos(a_px * PI * x / L) + p_y * sin(a_py * PI * y / L) + p_0) * rho_y * k * cos(a_rhoy * PI * y / L) * a_rhoy * a_rhoy * PI * PI * pow(r
ho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rhoy * PI * y / L) + rho_0, -0.2e1) * pow(L, -0.2e1) / R - (0.2e1 * p_x * cos(a_px * PI * x / L) + 0.2e1 * p_y * sin(a_py * PI * y / L) + 0.2e1 * p_0) *
 rho_y * rho_y * k * pow(sin(a_rhoy * PI * y / L), 0.2e1) * a_rhoy * a_rhoy * PI * PI * pow(rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rhoy * PI * y / L) + rho_0, -0.3e1) * pow(L, -0.2e1) / R + 
0.4e1 / 0.3e1 * mu * u_x * v_y * cos(a_ux * PI * x / L) * cos(a_vy * PI * y / L) * a_ux * a_vy * PI * PI * pow(L, -0.2e1) - 0.2e1 * mu * u_y * v_x * sin(a_uy * PI * y / L) * sin(a_vx * PI * x / L) * a
_uy * a_vx * PI * PI * pow(L, -0.2e1) - 0.2e1 * k * p_x * rho_x * cos(a_rhox * PI * x / L) * sin(a_px * PI * x / L) * a_px * a_rhox * PI * PI * pow(rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rho
y * PI * y / L) + rho_0, -0.2e1) * pow(L, -0.2e1) / R - 0.2e1 * k * p_y * rho_y * cos(a_py * PI * y / L) * sin(a_rhoy * PI * y / L) * a_py * a_rhoy * PI * PI * pow(rho_x * sin(a_rhox * PI * x / L) + r
ho_y * cos(a_rhoy * PI * y / L) + rho_0, -0.2e1) * pow(L, -0.2e1) / R - (v_x * cos(a_vx * PI * x / L) + v_y * sin(a_vy * PI * y / L) + v_0) * (rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rhoy * P
I * y / L) + rho_0) * (u_x * sin(a_ux * PI * x / L) + u_y * cos(a_uy * PI * y / L) + u_0) * v_x * sin(a_vx * PI * x / L) * a_vx * PI / L - Gamma * (u_x * sin(a_ux * PI * x / L) + u_y * cos(a_uy * PI *
 y / L) + u_0) * p_x * sin(a_px * PI * x / L) * a_px * PI / (Gamma - 0.1e1) / L + Gamma * (v_x * cos(a_vx * PI * x / L) + v_y * sin(a_vy * PI * y / L) + v_0) * p_y * cos(a_py * PI * y / L) * a_py * PI
 / (Gamma - 0.1e1) / L + k * p_x * cos(a_px * PI * x / L) * a_px * a_px * PI * PI / (rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rhoy * PI * y / L) + rho_0) * pow(L, -0.2e1) / R + k * p_y * sin(a
_py * PI * y / L) * a_py * a_py * PI * PI / (rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rhoy * PI * y / L) + rho_0) * pow(L, -0.2e1) / R;
  return(Q_e);
}
--:** NavierStokes_2d_e_code.C   All L11   SVN-9008  (C++/l Abbrev)----[61%]--------
Auto-saving...done
```

Additional Focus Areas

1. Physics Modeling
   - Weakly Ionized Flows
   - Surface Catalycity
   - Additional Boundary Conditions
2. Coupling
   - Radiation
   - Ablation
3. Adjoints
   - Sensitivity analysis
   - Adaptivity
4. Scalability

- Push range of applicability of code through internal NASA-JSC use this summer
- Perform PECOS full-system simulations using FIN-S as part of year 3 deliverables

Thank you!

Questions?