
A Newton-Krylov Based Solver for CFD Models Using Finite Rate NOx Chemistry

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Outline

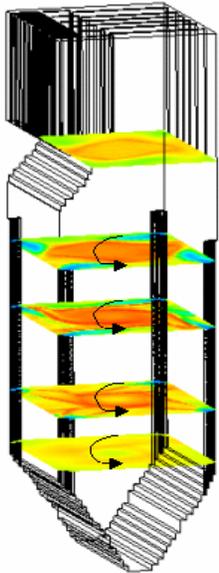
- Background
- Solution method
- Demonstrate basic solver on furnace configuration
- Recent Work
 - ◆ AMG Pre-conditioner
 - ◆ Reduced Mechanism Evaluation

Motivation

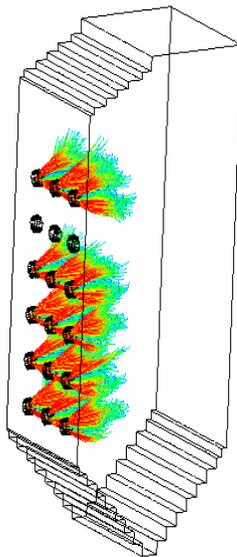
→ Modeling Finite Rate Chemistry effects in Chemically Reacting Flows is increasingly important for industrial applications

◆ pollutant emissions (Combustion + Incineration)

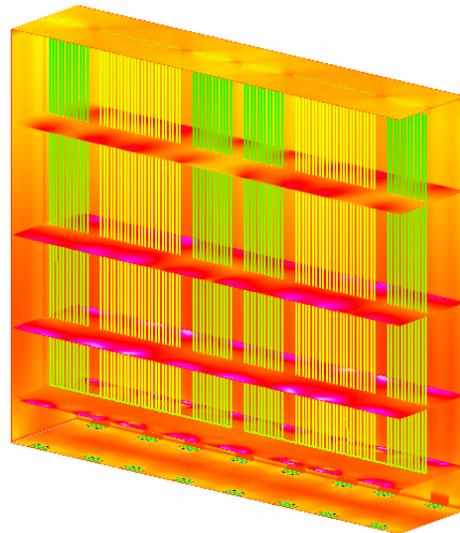
PC Fired



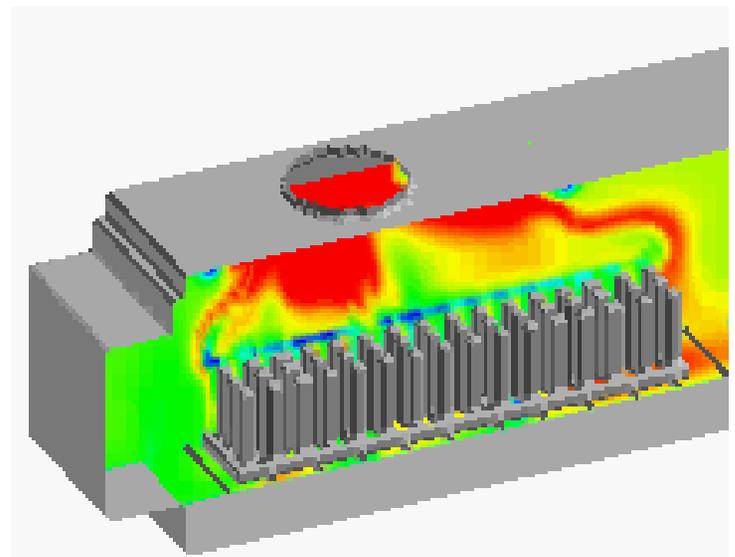
Oil-Fired



Process Heater



Incinerator



CFD Modeling & Finite Rate Chemistry

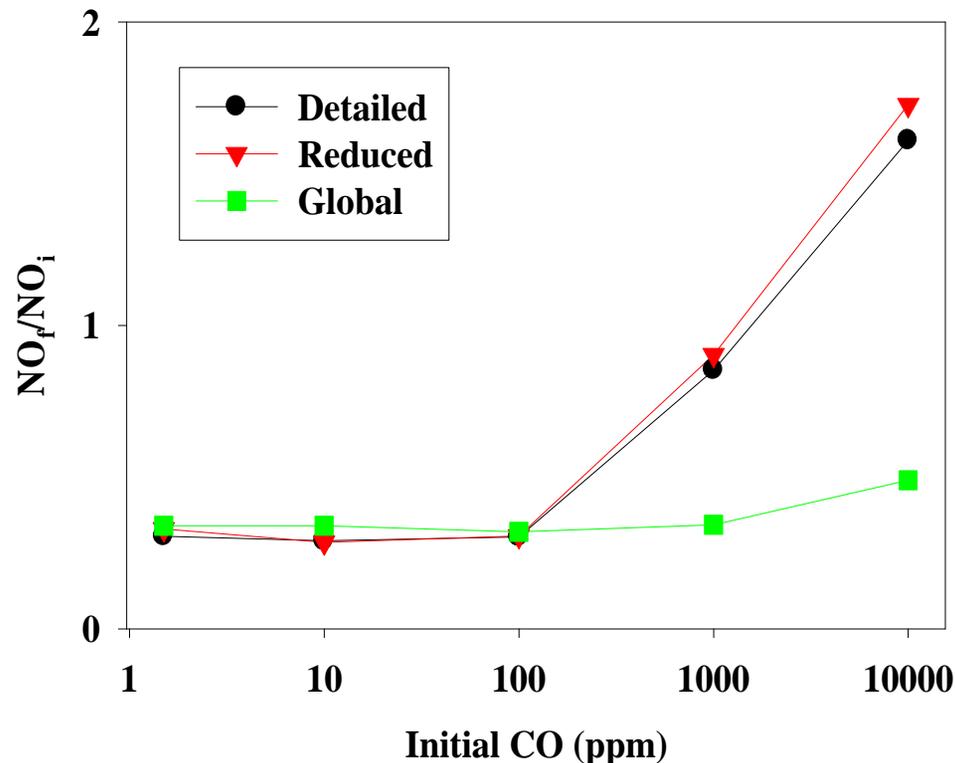
- Detailed
 - ◆ includes all known relevant reactions for process
 - ◆ accurate - but not practical for CFD
- Reduced
 - ◆ preserves accuracy of detailed mechanisms at reduced computational effort
 - » RCCE, ILDM, CSP, QSS [CARM],
 - ◆ limited range of applicability but more robust than global mechanisms
 - ◆ Induces Numerical stiffness
- Global

Complex,
Intractable

Simple,
Tractable

Example – NO_x Chemistry

compare detailed, reduced, and global chemistry



→ 10 specie reduced mechanism – CARM

◆ CARM developed by Prof. JYChen, UC-Berkeley

→ Detailed chemistry of Miller and Bowman (250 steps, 60 species)

→ Reduced Mechanism tracks Detailed Mechanism over wide range of temperatures, CO, O₂, initial NO

→ Global mechanism: 6 species, 7 reactions with explicit rate expression

Solution Scheme - Overview (1)

Assume heat release for non-equilibrium reactions small relative to overall combustion

- combustion flow field not effected by non-equilibrium reactions

Split problem into two *manageable* steps:

1. solve equilibrium combustion flow field → gas velocity, density, temperature, major species, ...
2. compute trace species based on non-equilibrium reactions as a post-processor

Iteratively solve transport equations for non-equilibrium chemical species

$$\nabla (\overline{\mathbf{r}\mathbf{u}} \overline{\mathbf{x}}_i) + \nabla (\text{De} \nabla \overline{\mathbf{x}}_i) = \overline{\mathbf{w}}_i(\overline{\mathbf{x}})$$

Discrete form:

$$A_p x_p - \sum A_{nb} x_{nb} = S_u + S_p x_p^*$$

chemistry model
determines sources

Solution Scheme - Overview (2)

Solution Procedure

- initialize X_p
- update chemical source terms
 - global or skeletal mechanism => analytic expression
 - reduced mechanism => FORTRAN expression
- solve for new X_p
 - solve transport equations sequentially
 - ✓ Original Method → Picard
 - ✓ New Method → Newton-Krylov
- converged ?

Matrix Free Newton-Krylov Solver (1)

- Reformulate outer iteration loop for Newton Method

$$\mathbf{F}(\mathbf{x}^k) + \mathbf{J} \times \mathbf{s}^k = 0$$

where

$$\mathbf{F}(\mathbf{x}) = [f_1(\mathbf{x}), \dots, f_n(\mathbf{x})]^T$$

$$f(x_p) = A_p x_p - \sum A_{nb} x_{nb} - (S_u + S_p x_p^*)$$

$$\mathbf{J} = \text{Jacobian} = \mathbf{F}'(\mathbf{x}^k) = [\partial F_i / \partial x_j],$$

$$\mathbf{s}^k = \text{solution step} = (\mathbf{x}^{k+1} - \mathbf{x}^k)$$

- Inexact Newton Method to update solution step

$$\|\mathbf{F}(\mathbf{x}^k) + \mathbf{J} \times \mathbf{s}^k\| \leq \mathbf{h}^k \|\mathbf{F}(\mathbf{x}^k)\|, \quad \mathbf{h}^k = \text{forcing term} \leq 1$$

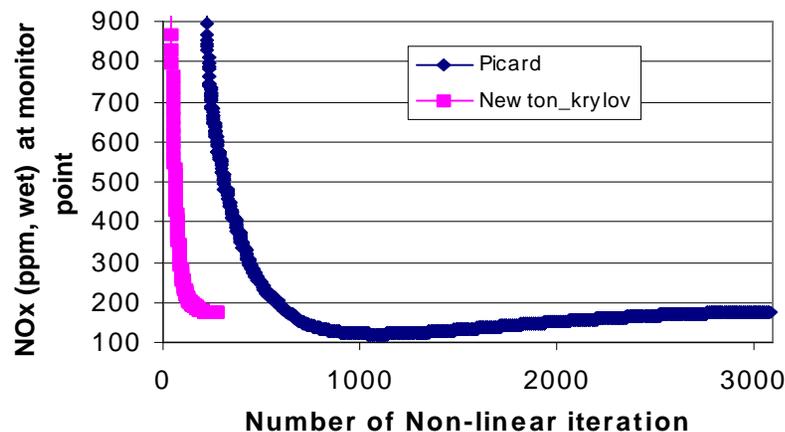
Matrix Free Newton-Krylov Solver (2)

- GMRES for inner iteration to update s^k
- matrix free formulation: J never explicitly formed
- approximate matrix vector product with finite difference:
 - requires only one additional residual evaluation $J \times s^k = \frac{F(x^k + e, s^k) - F(x^k)}{e}$
- Reduced Mechanism requires pre-conditioner in GMRES
- solve system of form $M \times z = r$
 - where M = pre-conditioner, r = Newton method residual
- pre-conditioner defined with “frozen coefficients” from discrete operators
 - convection / diffusion operator contributions known from outer iteration loop
 - chemical source term derivative contributions approximated with linearization
- pre-conditioner matrix never explicitly formed
- s^k obtained from $M \times s = z$ with Gauss-Seidel iteration

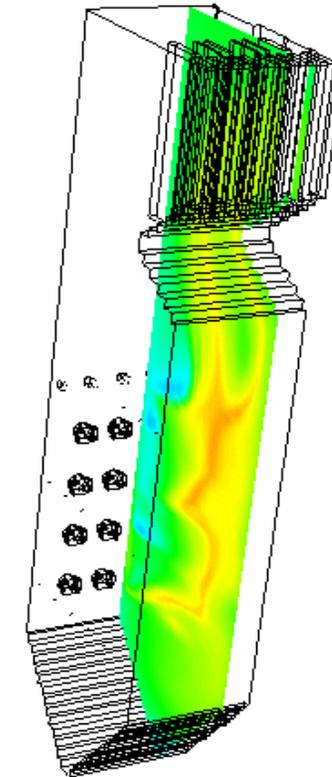
Results

- up to 60% speed up for full scale coal fired utility boiler NOx simulations
- Improved robustness & ease of use
- Greater improvement on more difficult problems

Case	Reduced Mechanism	Grid Size	% CPU Reduction
550 Mwe wall fired utility boiler w/SNCR (upper furnace only)	10 species NOx-SNCR	538 K	48
138 Mwe cyclone fired furnace w/OFA	10 species NOx-SNCR	425 K	56
177 MWe wall fired utility boiler	13 speices NOx	513 K	62



177 MWe
Wall Fired
Utility Boiler



Work In Progress

Algebraic Multi-Grid Pre-conditioner

Algebraic Multi-Grid (AMG) Pre-conditioner

→ Motivation

- ◆ Reduce cpu effort and increase robustness

→ AMG

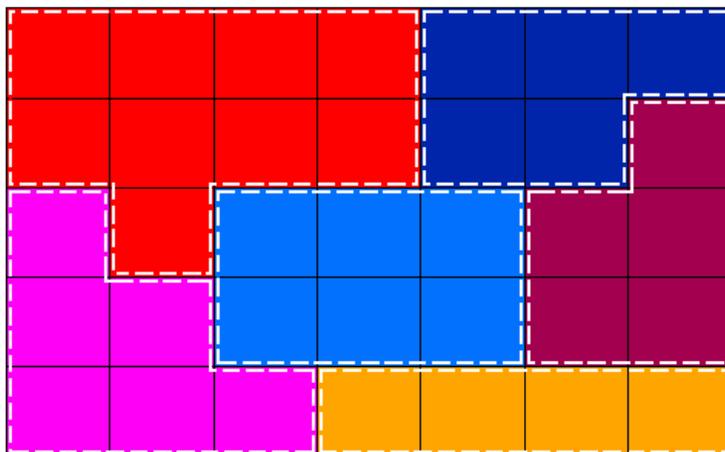
- ◆ Might not be “optimal” MG method...
- ◆ BUT
 - » Amenable to block structured grid with imbedded boundaries and complicated geometry such as for industrial applications
 - » Potential to also use on unstructured (AMR) grid
 - » Flexible => want 1 code to work in many situations

→ Approach

- ◆ Re-use an AMG solver developed by REI for an Adaptive Mesh Refinement (AMR) flow solver
 - » AMG solver has been used for “isothermal” gas flow and (limited) combustion applications
- ◆ Use as a “Black Box”
- ◆ AMG → “Aggregation” AMG

AMG

- Coarse grid problem created from discretized eqns, NOT geometry
- Coarse cells created by grouping contiguous fine cells
 - ◆ minimum number of cells in each group is preset (8 for 3D)
 - ◆ cells added to “group” to create maximum coupling (based on neighbor coefficients)
 - ◆ for “frozen” coefficient approach → only build list of cells for each group one time
- Coarse grid equations are assembled by adding coefficients & source terms from the fine grid



- Can result in “odd” shaped coarse cells
- Arbitrary levels of coarsening allowed

———— Fine cell boundaries (level h)
- - - - Coarse cell boundaries (level H)

AMG Cycle

- V cycle
 - ◆ Arbitrary levels of coarse grid
- Direct solve on the coarsest grid
 - ◆ If system too large, can use iterative solve
- Smoother
 - ◆ point gauss siedel
 - ◆ “line solve” available, but not used
 - » In the AMR CFD solver, use of AMG to solve for velocity, pressure, etc has eliminated need for line solver

Preliminary Results - HotBox

Note:

- Spheres = urea injection ports
- Streaks = droplet trajectories
- Planes = gas temperature

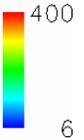
10 species NO_x-SNCR
reduced mechanism

combustion
products

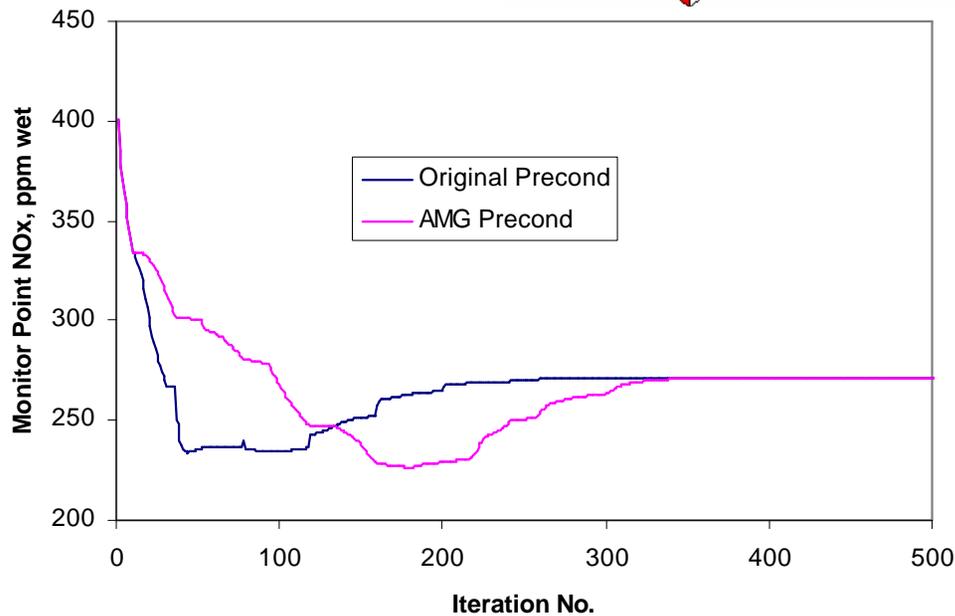
INLET

Gas
Temperature

OUTLET



NO_x



**AMG Preconditioner “works”
but needs “tuning” to realize benefits**

Recent Work

Reduced Mechanism Evaluation

Reduced Mechanism Evaluation

→ Motivation

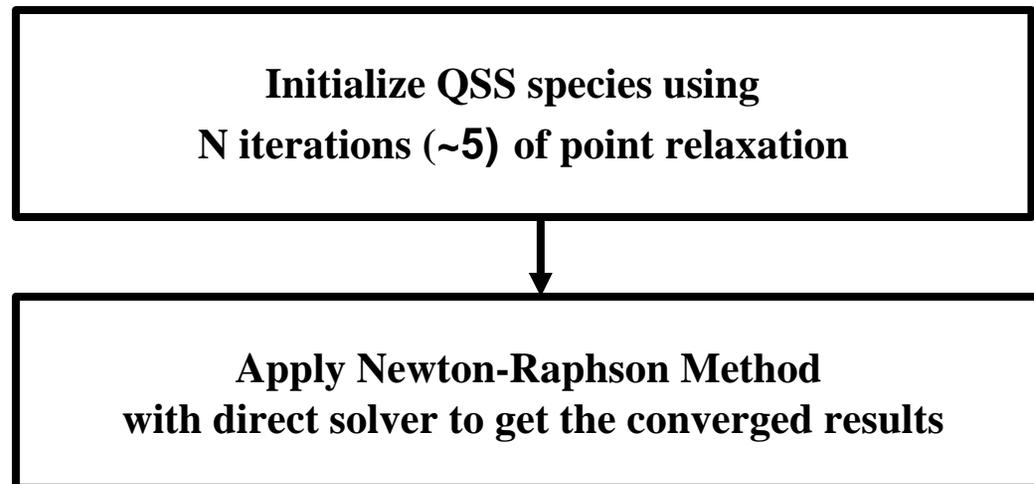
- ◆ For Newton Krylov solver, ~40-50% of cpu time consumed in solution of non-linear algebraic equations that determine QSS species in reduced mechanism
 - » Needed to evaluate jacobian
- ◆ Can fail to converge ~10% of cells

→ Original Method

- ◆ Solve for QSS with point iteration (~gauss siedel iteration for linear system)
- ◆ Ambiguities in definition of stopping criteria
- ◆ Slow convergence rate
 - » 10's → 100's of iterations required
- ◆ Point iteration method convergence can “stall” → incorrect source terms handed back to main solver
 - » Contribute to numerical stiffness
 - » Can lead to incorrect overall solution

Improvements

- A Combined nonlinear equation solver for QSS species :
 - point iteration and Newton-Raphson iteration



- New Stop Criteria:

$$\mathbf{e} \equiv \left| N_j^{n+1} - N_j^n \right| \leq \max \left(N_j^{n+1} \cdot \mathbf{e}_{Rtol}, \mathbf{e}_{Atol} \right), \quad \text{for } j = 1, \dots, n_s$$
$$n \leq n_{\max}$$

Where N_i = the concentration of QSS species i

Test Cases

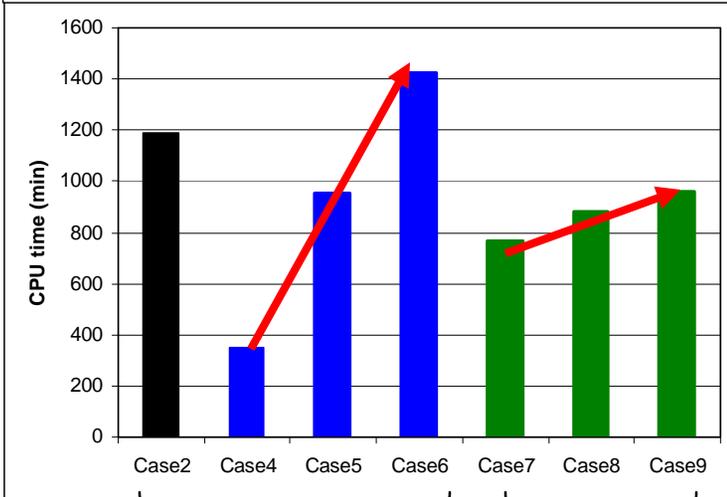
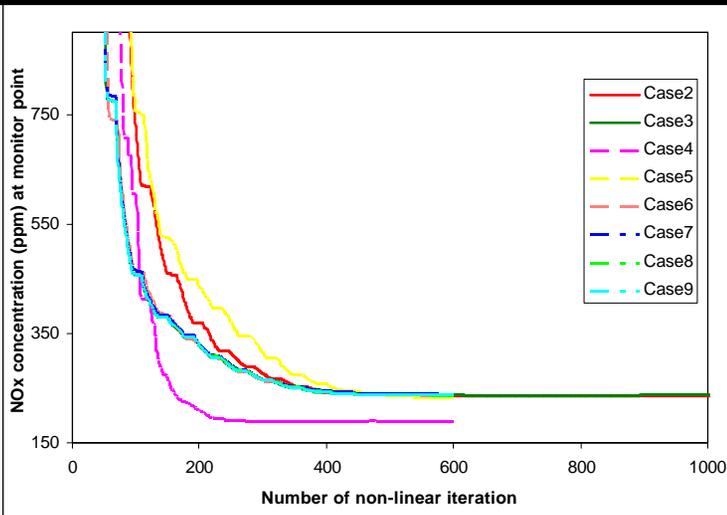
➤ Reduced mechanism

- 10 non-steady state species: CO₂, CO, O₂, OH, H₂O, N₂, NO, N₂O, HNCO, NH₃
- 16 steady state species: NCO, N, NH₂, NH, NNH, HOCN, HNO, H, O, HCN, HCNO, HO₂, H₂O₂, H₂, NO₂

➤ Test Cases

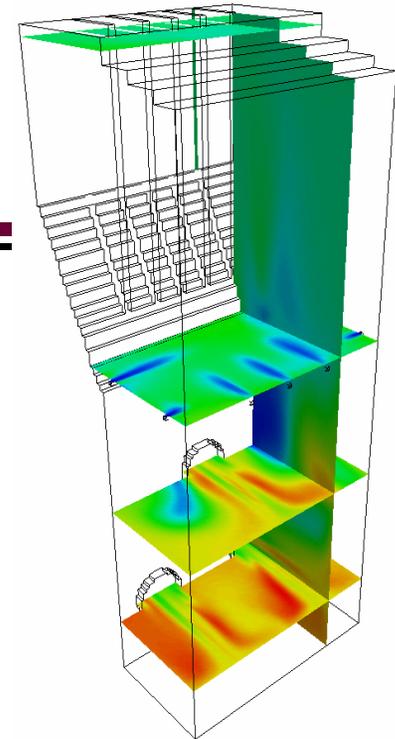
Case index	Stop Criteria	Solver
1	Old stop criteria, $n_{\max} = 25$, $e = 10^{-5}$	Point iteration
2	Old stop criteria, $n_{\max} = 200$, $e = 10^{-5}$	Point iteration
3	New stop criteria, $n_{\max} = 200$, $e_{Atol} = 10^{-15}$, $e_{Rtol} = 10^{-9}$	Point iteration + Newton Raphson
4	New stop criteria, $n_{\max} = 200$, $e_{Atol} = 10^{-9}$, $e_{Rtol} = 10^{-3}$	Point iteration
5	New stop criteria, $n_{\max} = 200$, $e_{Atol} = 10^{-12}$, $e_{Rtol} = 10^{-6}$	Point iteration
6	New stop criteria, $n_{\max} = 200$, $e_{Atol} = 10^{-15}$, $e_{Rtol} = 10^{-9}$	Point iteration
7	New stop criteria, $n_{\max} = 200$, $e_{Atol} = 10^{-9}$, $e_{Rtol} = 10^{-3}$	Point iteration + Newton Raphson
8	New stop criteria, $n_{\max} = 200$, $e_{Atol} = 10^{-12}$, $e_{Rtol} = 10^{-6}$	Point iteration + Newton Raphson
9	New stop criteria, $n_{\max} = 200$, $e_{Atol} = 10^{-15}$, $e_{Rtol} = 10^{-9}$	Point iteration + Newton Raphson

Results – Cyclone Fired Boiler



Point iteration

Newton Raphson



Point Relaxation for QSS:

- Needs $O(100)$ iterations to ensure convergence
- rapid increase in cpu effort for tighter tolerance
- Incorrect “stopping” criteria
 → QSS solver stalls often → incorrect solution

Newton Raphson for QSS:

- modest increase in cpu effort for tighter tolerance
- larger tolerance results in same solution
- modest improvement in cpu time vs. Point method
- QSS solver always converges

Similar findings for HotBox and Lean SNCR Utility Boiler cases

Future Work

- ➔ Continue to Improve Newton Krylov CFD solver
 - AMG pre-conditioner
 - reduced mechanism evaluation
 - problem initialization

- ➔ Demonstrate for low NOx simulations
 - Coal combustion – electric utility boilers
 - Gas combustion – chemical process furnaces

Acknowledgments

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Questions, Comments, Suggestions.....
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