THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

Application of a Jacobian-Free Newton-Krylov Method to the Simulation of Hypersonic Flows

Kyle Damm, Nicholas Gibbons, Peter Jacobs and Rowan Gollan

Centre for Hypersonics

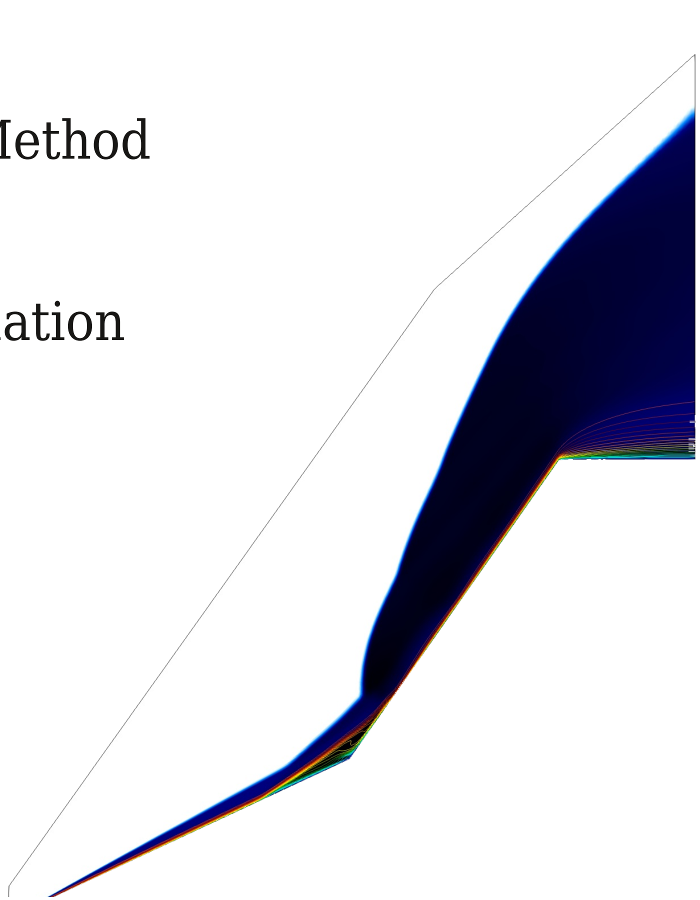
School of Mechanical & Mining Engineering

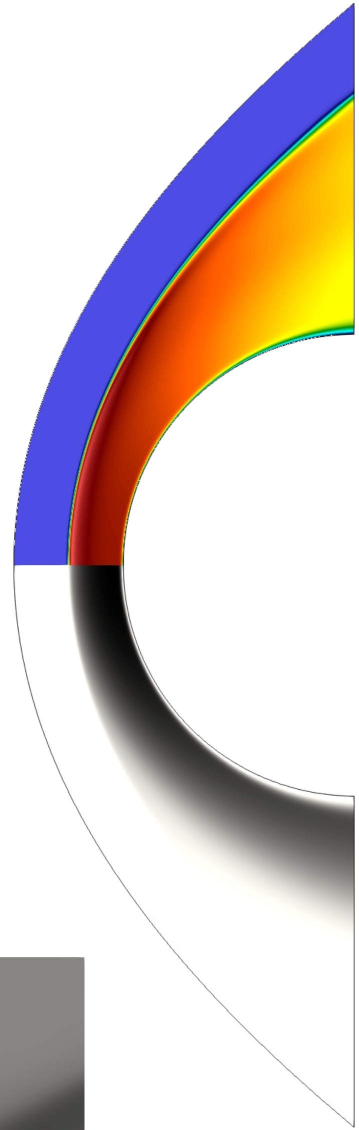
The University of Queensland, Australia

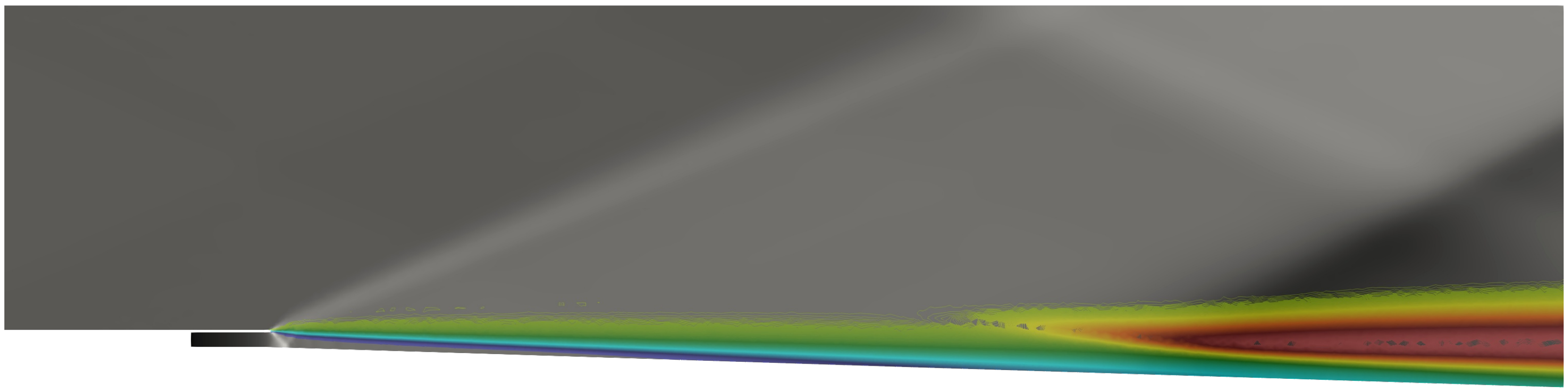
AIAA SciTech Forum, National Harbor MD, 23 -- 27 January 2023

Outline

- Context: Eilmer flow solver
- Jacobian-free Newton-Krylov Method
    - + Newton method
    - + pseudo-transient continuation
    - + Krylov method: GMRES
- Point-implicit relaxation
- Performance comparisons



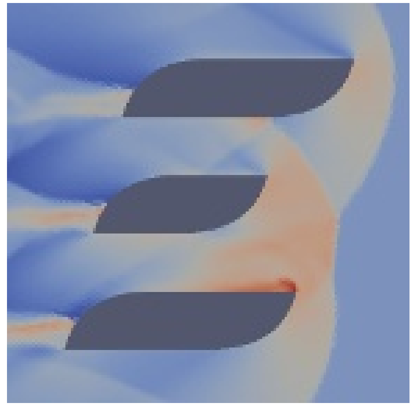


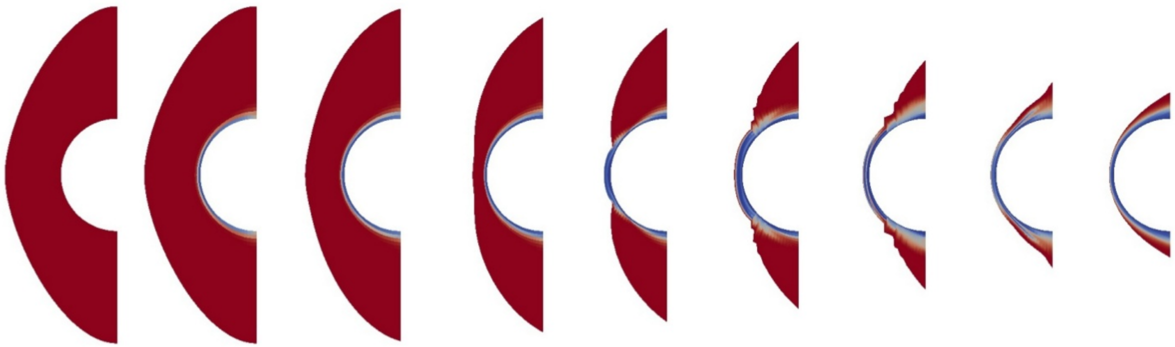


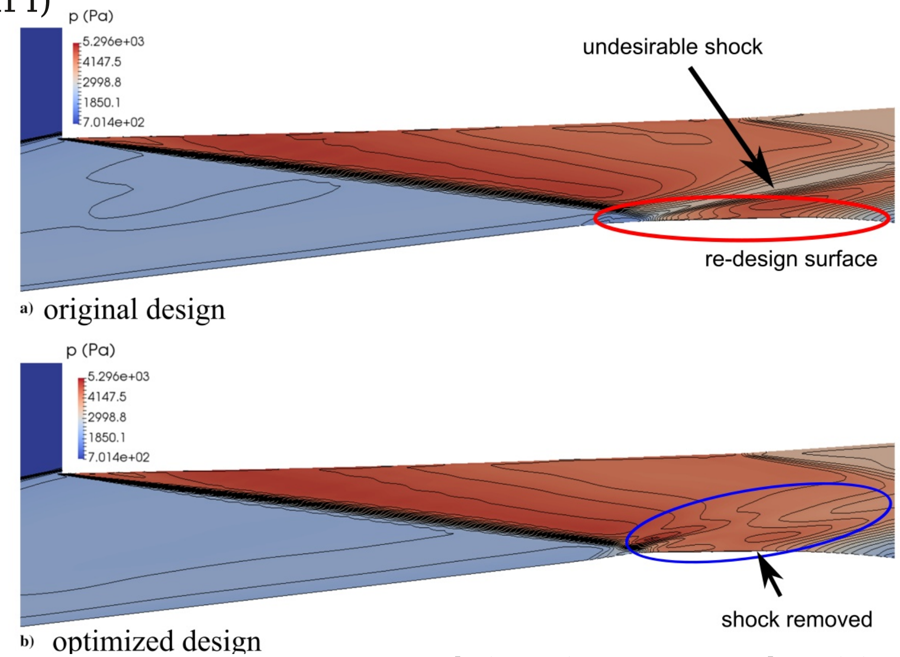
Eilmer: what it does

THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

+ 2D/3D compressible flow simulation
+ Gas models include ideal, thermally perfect, multi-temperature and state-specific
+ Finite-rate chemistry
+ Inviscid, laminar, turbulent flows
+ Solid domains with conjugate heat transfer
+ User-controlled moving grid capability
+ Shock-fitting method for blunt body show layers
+ A rotating frame of reference for turbomachine modelling
+ Transient, time-accurate updates with Runge-Kutta family integrators
+ Steady-state accelerator using Newton-Krylov approach
+ User-defined customisations available for boundary conditions, source terms, and pre- and post-processing
+ Parallel computation using shared memory or distributed memory (MPI)
+ Multiple-block structured and unstructured grids
+ Native grid generation and 3rd-party import capability
+ Unstructured-mesh partitioning via Metis
+ Adjoint solver for efficient sensitivies evaluation







Damm et al. (2020) AIAA Journal, 58(6)

`Eilmer`: how it works

THE UNIVERSITY OF QUEENSLAND AUSTRALIA

solves the compressible Navier-Stokes equations with multi-species multi-temperature extensions

$$\frac{\partial}{\partial t}\int_V \mathbf{U}\, dV = -\oint_S (\mathbf{F}_i - \mathbf{F}_v)\cdot\hat{n}\, dA + \int_V \mathbf{Q}\, dV$$

$$\mathbf{U} = \left[\rho v_x, \rho v_y, \rho v_z, \rho E, \ldots, \rho_s, \ldots, \rho e_v\right]^T$$

using finite volume discretization

$$\frac{\partial \mathbf{U}}{\partial t} = -\frac{1}{V}\sum_f^{\text{faces}} (\mathbf{F}_i - \mathbf{F}_v)_f \cdot \hat{n}_f\, A_f + \mathbf{Q} = \mathbf{R}(\mathbf{U})$$

Residual evaluation:

1. Reconstruct the flow on both sides of each face
2. Compute the inviscid fluxes $\mathbf{F}_i$
3. Compute the gradients of the flow at each face
4. Compute the viscous fluxes $\mathbf{F}_v$
5. Compute the source term $\mathbf{Q}$ in each cell
6. Compute the residual $\mathbf{R} = \partial\mathbf{U}/\partial t$

The promise of JFNK...

handle any selection of options
for R(U) automatically

Jacobian-free Newton-Krylov Overview

Newton method

$$\left(\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right)^n \Delta \mathbf{U}^n = -\mathbf{R}(\mathbf{U}^n), \qquad \mathbf{U}^{n+1} = \mathbf{U}^n + \Delta \mathbf{U}^n, \qquad n = 0, 1, \ldots.$$

Krylov method

+ iterate to solve a linear system

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

Jacobian-free

+ never form Jacobian explicitly
+ find algorithm that only uses Jacobian-vector products

Pseudo-transient continuation

to help get into the region of convergence, step loosely in time

$$[\mathbf{A}]^n \Delta \mathbf{U}^n = \left\{ \frac{1}{\Delta t_{\text{local}}} \mathbf{I} - \frac{\partial \mathbf{R}^n}{\partial \mathbf{U}} \right\} \Delta \mathbf{U}^n = \mathbf{R}^n.$$

and solve this system inexactly

$$||\mathbf{R}^n - [\mathbf{A}]^n \Delta \mathbf{U}^n|| \leq \eta ||\mathbf{R}^n||$$

as the residual drops, grow the CFL to recover Newton's method

$$CFL^n = CFL^{n-1} \left(\frac{||\mathbf{R}(\mathbf{U}^{n-1})||}{||\mathbf{R}(\mathbf{U}^n)||} \right)^a$$

to add further robustness, use a relaxation factor based on a physicality check

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \omega^n \Delta \mathbf{U}^n \qquad \text{with:} \quad 0 < \omega^n \leq 1$$

adjust ω^n so that:

- change in species mass is not too large
- primitive values are physically realizable

Krylov method

THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

We use **GMRES**: Generalized Minimum RESidual iterative solver:

- **Jv** – only matrix-vector products appear
- strong solve – via global dot product
- registers of memory scale linearly with number of Krylov vectors

Fréchet derivative using complex number:

$$\mathbf{J}\mathbf{v} \approx \frac{\mathrm{Im}[\mathbf{R}(\mathbf{U} + h\mathbf{v}i)]}{h}.$$

Point-implicit relaxation

$$[\mathbf{A}]^n \Delta\mathbf{U}^n = \left\{ \frac{1}{\Delta t_{\mathrm{local}}}\mathbf{I} - \frac{\partial \mathbf{R}^n}{\partial \mathbf{U}} \right\} \Delta\mathbf{U}^n = \mathbf{R}^n.$$

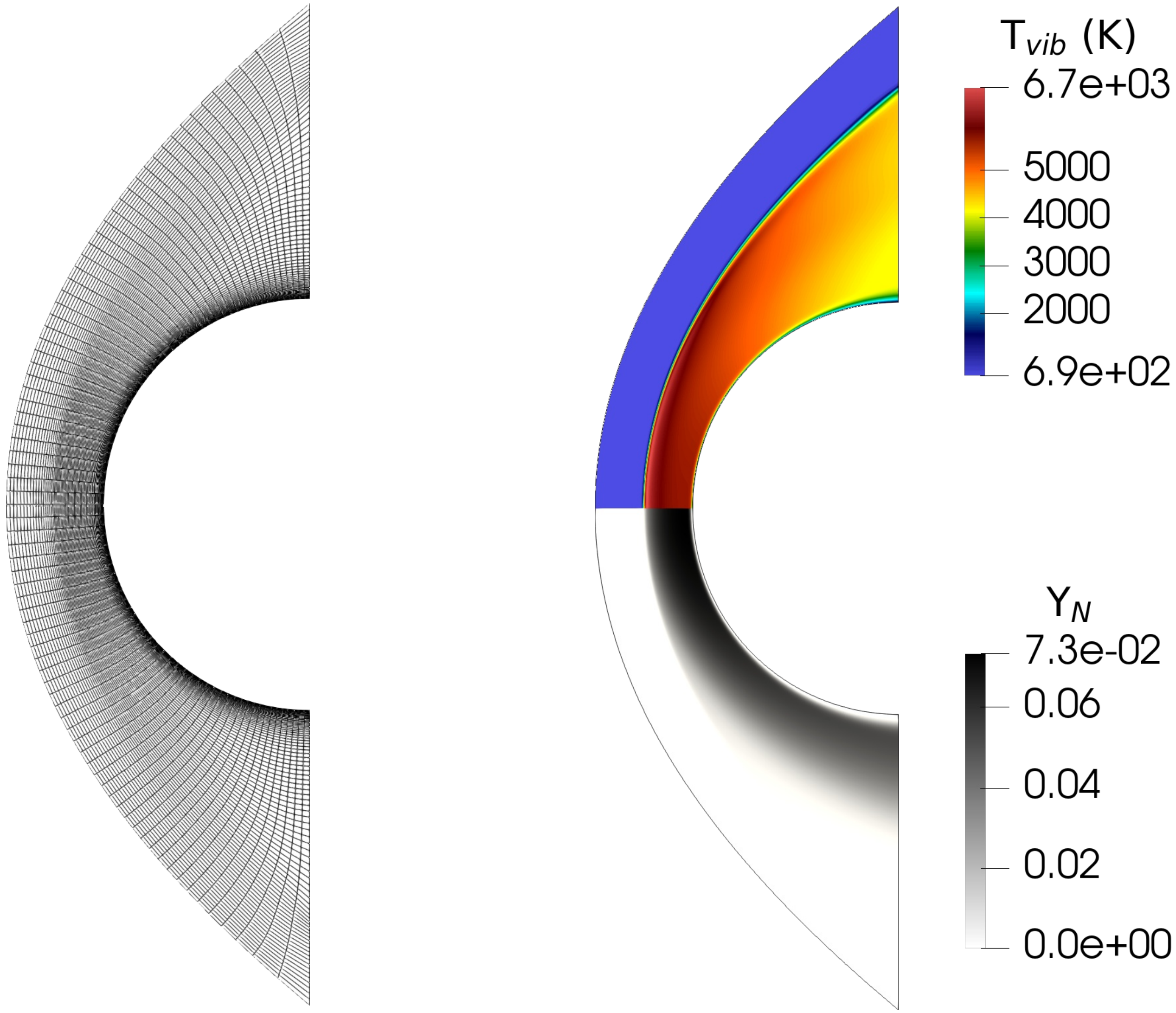
A defect correction type update:

- Jacobian per cell; local effects only
- first-order spatial reconstruction

Other notes:

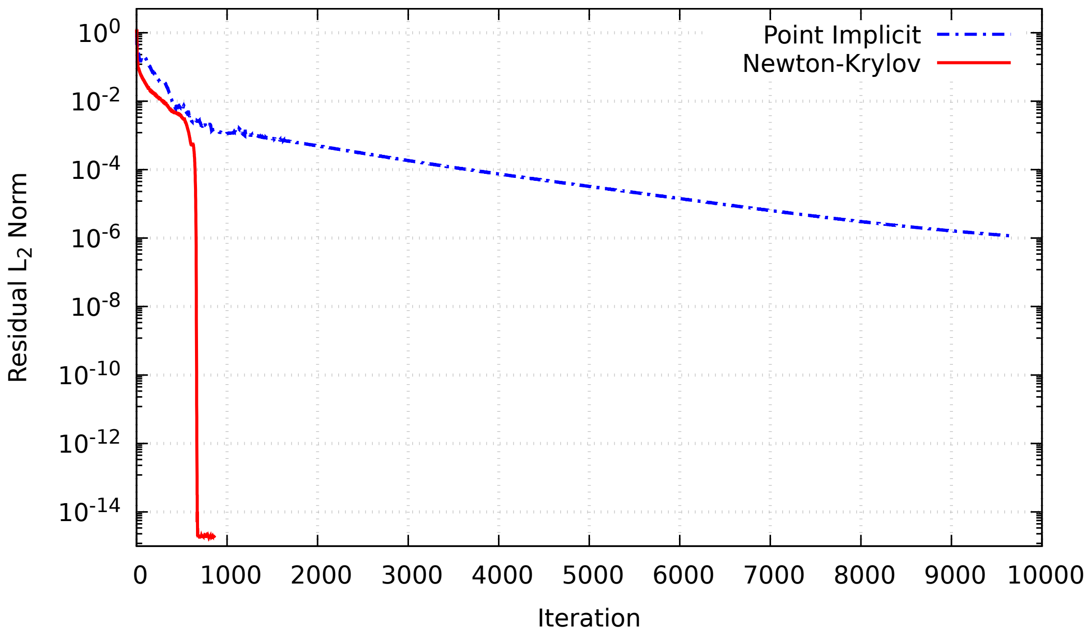
- local Jacobian formed using complex-step perturbations
- direct solve to give update

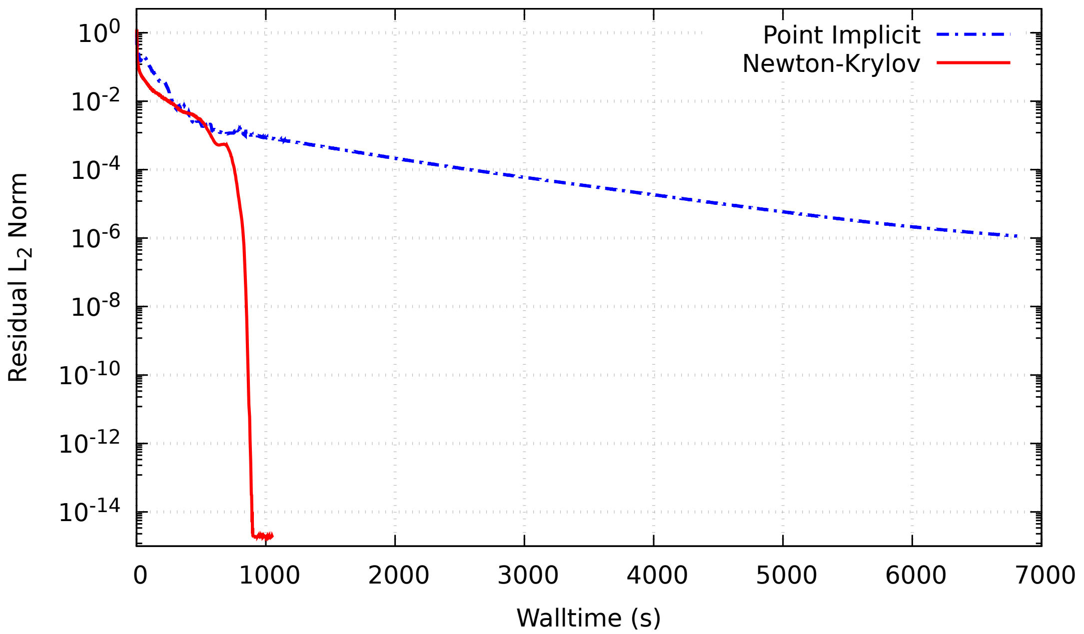
High-enthalpy cylinder flow: description



- air flow over $R = 45\,\mathrm{mm}$ cylinder
- free-stream enthalpy: 13.5 MJ/kg
- Park 2-T model
- Fickian diffusion

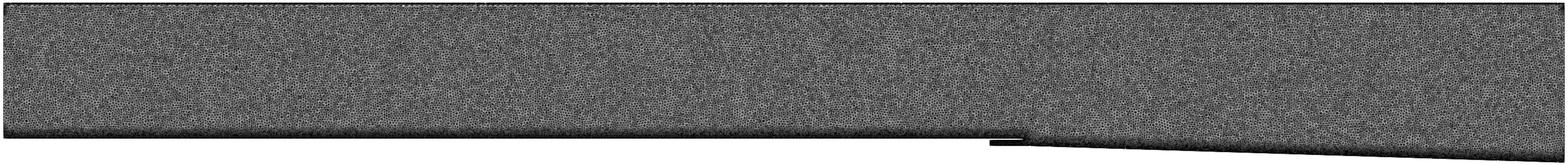
High-enthalpy cylinder flow: results

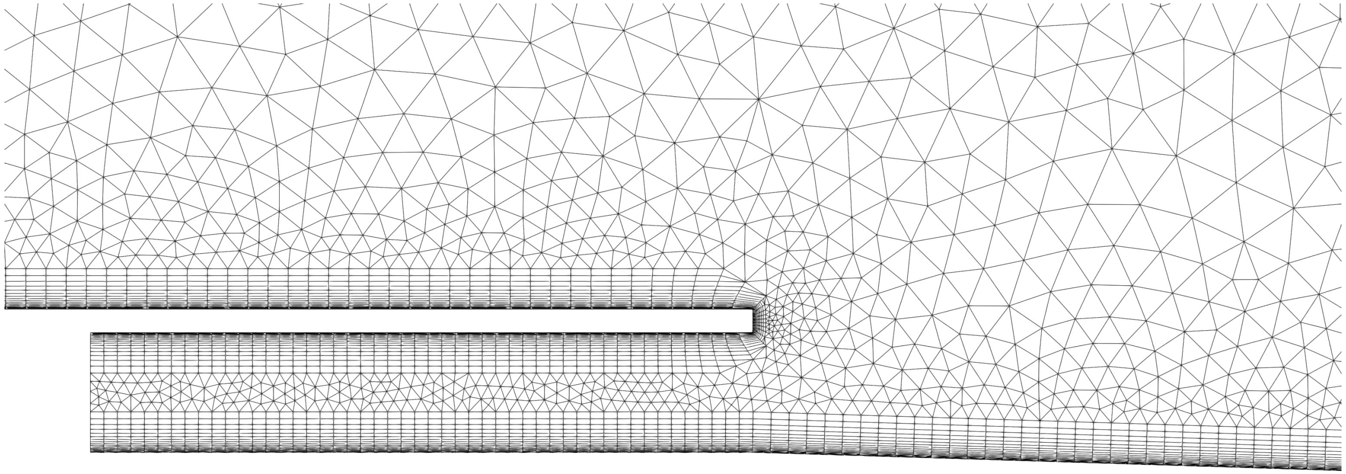




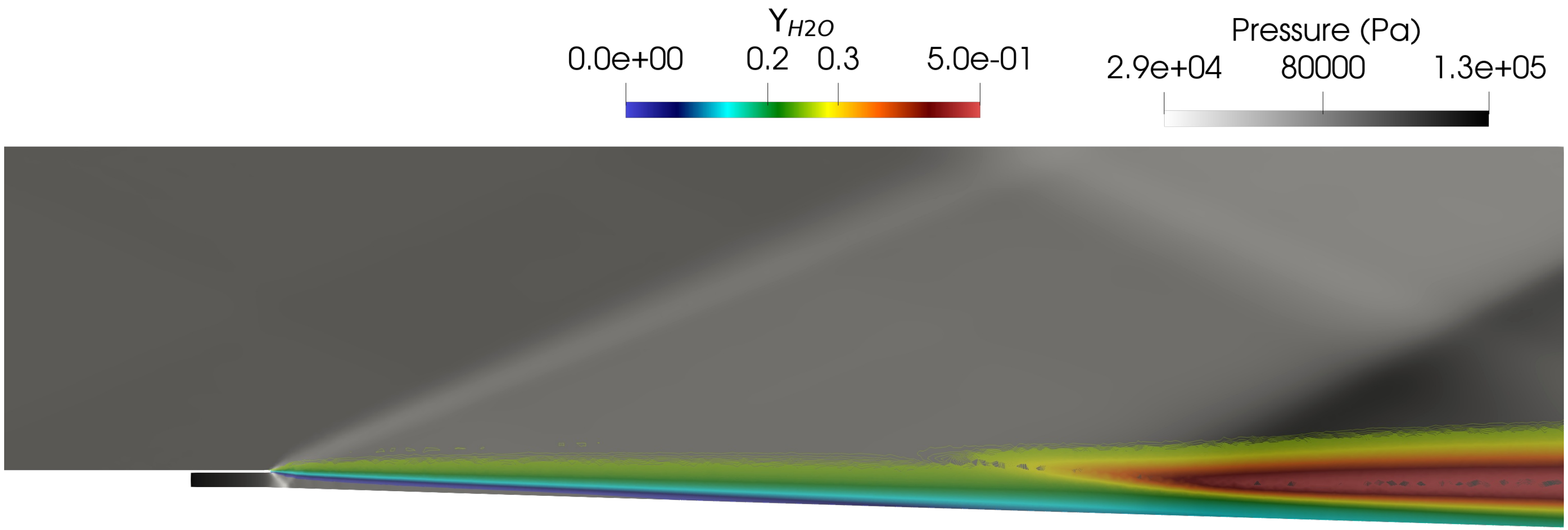
Supersonic combustor: description

THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

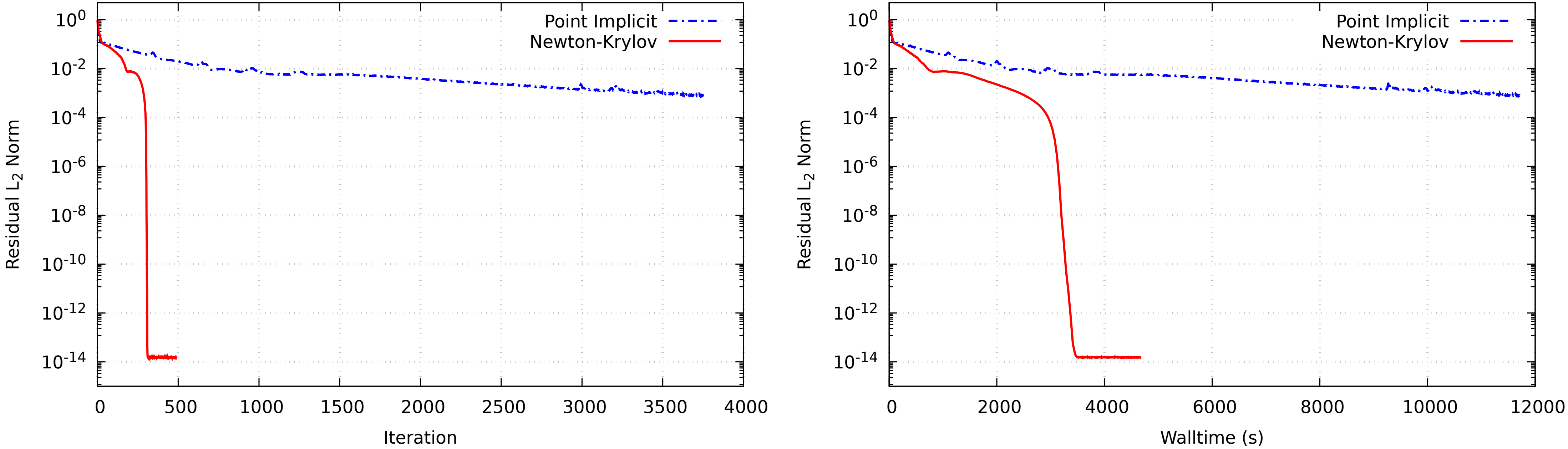




- main stream: vitiated air
- injected stream: hydrogen
- mixture of thermally perfect gas
- Evans-Schexnayder 7×8 H_2-air combustion



Supsersonic combustor: results



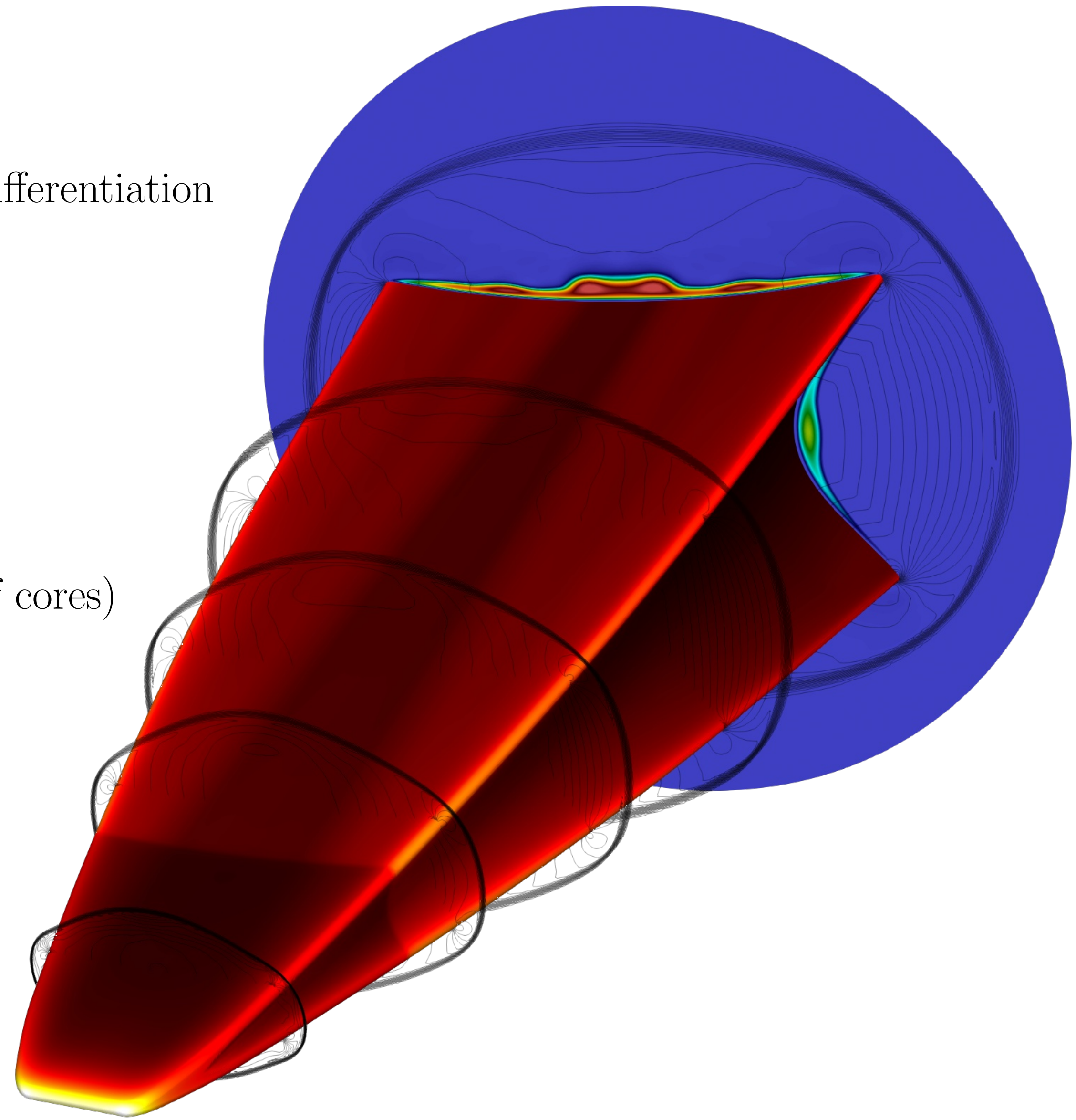
Concluding remarks

Summary

- JFNK provides deep convergence for multi-species multi-temperature hypersonic flows
- Key enablers are:
  - GMRES
  - Fréchet derivative with complex-number differentiation
- outperforms a point-implicit relaxation

Outlook

- method works well in 3D, but
- needs performance optimization / algorithm enhancements at large scale (1000s of cores)



Backup 1: effect of preconditioner selection

THE UNIVERSITY OF QUEENSLAND AUSTRALIA