

Simulating Re-entry flows with Eilmer 4

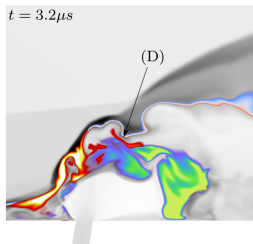
Nick N. Gibbons,
The University of Queensland, Brisbane, Queensland 4072, Australia

July 21, 2021

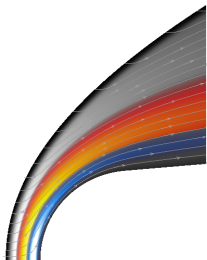
About Me!

- ▶ Undergraduate degree in Aerospace Engineering at UQ (2010-2013)
- ▶ PhD in Supersonic Turbulent Combustion also at UQ (2014-2019)
 - ▶ Supervised by Prof. Vincent Wheatley and Dr. Alexander Klimenko
- ▶ Postdoctoral Research Fellow (2020-present)
 - ▶ Supervised by Dr. Rowan Gollan
 - ▶ Linkage project with Lockheed Martin Australia on Electron Transpiration Cooling

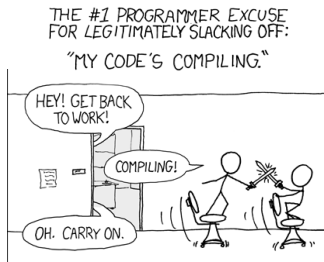
- ▶ Research Things I Do:



Supersonic Turbulent
Combustion



Hypersonic Plasma Flows

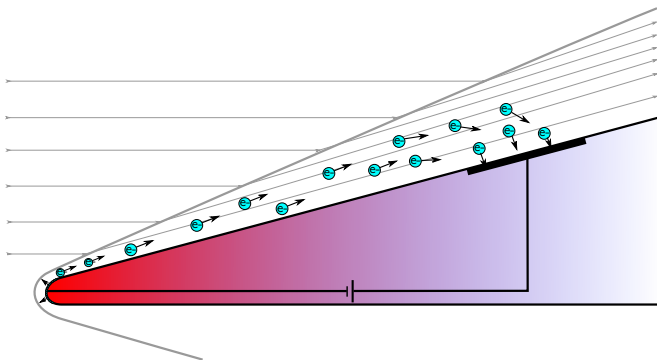


Parallel Programming for HPC

- ▶ You can follow me on Twitter! (@DrNickNGibbons)

Electron Transpiration Cooling

- ▶ Electrons take energy away from the surface and cool the emission point
- ▶ Surfaces can be sharp, compared to internal active cooling
- ▶ Need temperature/oxidation resistant material with low work function Φ



Eilmer4: An Open Source Compressible Fluid Solver

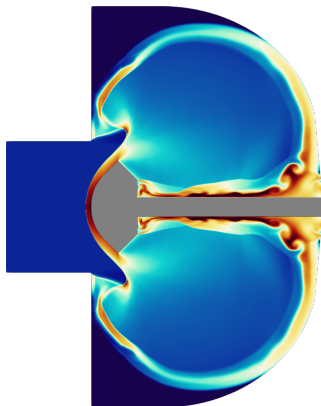
- ▶ Eilmer4 is our flagship compressible fluid dynamics code
- ▶ Freely available under the GPL 3.0 license (<https://gdtk.uqccloud.net/>)

Features:

- ▶ 2D/3D Structured or Unstructured grids
- ▶ Parallel scaling to thousands of cores
- ▶ RANS turbulence modelling
- ▶ Chemical reactions and multi-temperature flow
- ▶ Build your own grids or import them from common formats
- ▶ Extensively tested against data from hypersonics experiments

Experimental Features:

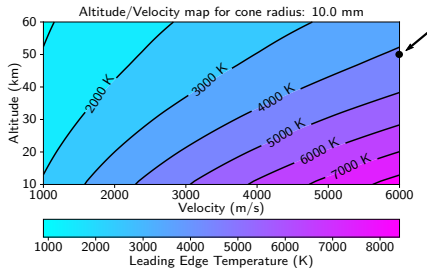
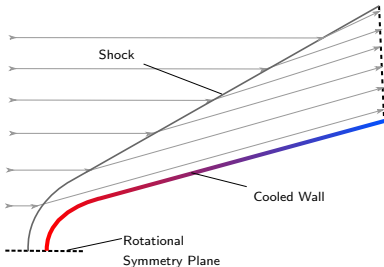
- ▶ Steady-state accelerator
- ▶ Low-dissipation fluxes for DNS/LES
- ▶ Lots of other things...



Eilmer4 solution of expansion tube over the Muses-C aeroshell, by Peter Jacobs.

Example Simulation: Uniform

- ▶ Work-in-progress simulations for AIAA ASCEND conference in November
- ▶ Blunt cone ($r = 10\text{mm}$) with cooled wall at $v = 6000\text{m/s}$ and $h = 50\text{km}$
- ▶ Compute leading edge temperatures for Radiation only versus Radiation+ETC
- ▶ Electron Transpiration Cooling model from Alkandry, Hanquist, and Boyd, 2014
- ▶ Convective heating estimates from correlation by Brandis and Johnston, 2014

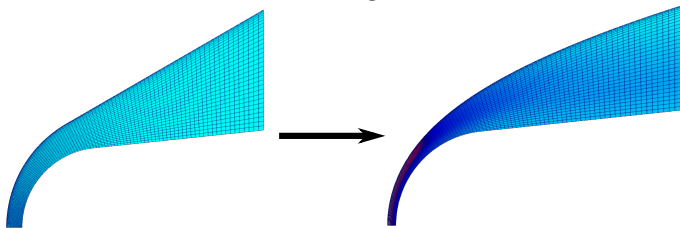


Solving Reentry Flows

► Workflow:

1. Inviscid, shock fitting simulation to establish shock shape
2. Extract shock boundary and regrid with clustering
3. Coarse viscous solution with steady state solver
4. Fine viscous solution with steady state solver

Shock Fitting Procedure:



Example Script: Core Simulation Parameters

Contents of input file etc.lua:

```
1  -- Simulation of ETC cooled cones phase 2: e4-nk-dist viscous solve
2  --
3  -- @author: Nick N. Gibbons
4  -- 2021-06-25
5
6  job_title = "Blunt Cone Shock Fitting"
7  config.dimensions = 2
8  config.axisymmetric = true
9  config.viscous = true
10
11 config.flux_calculator = "hanel"
12 config.spatial_deriv_locn = "cells"
13 config.spatial_deriv_calc = "least_squares"
14
15 config.mass_diffusion_model = "ficks_first_law"
16 config.diffusion_coefficient_type = "binary_diffusion"
...
129
```

Example Script: Numerical Method Options

```
1  -- Simulation of ETC cooled cones phase 2: e4-nk-dist viscous solve
2  --
3  -- @author: Nick N. Gibbons
4  -- 2021-06-25
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6  job_title = "Blunt Cone Shock Fitting"
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14
15 config.mass_diffusion_model = "ficks_first_law"
16 config.diffusion_coefficient_type = "binary_diffusion"
...
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```


Example Script: Species Diffusion Options

```
11 config.flux_calculator = "hanel"
12 config.spatial_deriv_locn = "cells"
13 config.spatial_deriv_calc = "least_squares"
14
15 config.mass_diffusion_model = "ficks_first_law"
16 config.diffusion_coefficient_type = "binary_diffusion"
17
18 nsp, nmodes, gmodel = setGasModel('gm-air11-2T.lua')
19 config.reactng = true
20 config.reactions_file = 'rr-kim-air11-2T.lua'
21 config.energy_exchange_file = 'ee-kim-air11-2T.lua'
...
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```

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} (\rho_s u_j) + \frac{\partial}{\partial x_j} D_s \frac{\partial Y_s}{\partial x_j} = \dot{\omega}_s \quad (1)$$

Example Script: Gas, Chemistry, and Energy Exchange

```
15 config.mass_diffusion_model = "ficks_first_law"
16 config.diffusion_coefficient_type = "binary_diffusion"
17
18 nsp, nmodes, gmodel = setGasModel('gm-air11-2T.lua')
19 config.reactng = true
20 config.reactions_file = 'rr-kim-air11-2T.lua'
21 config.energy_exchange_file = 'ee-kim-air11-2T.lua'
22
23 T_inf = 270.65      -- K
24 rho_inf = 0.000977521752421559  -- kg/m^3
25 mass_fraction = {N2=0.767, O2=0.233}
26 u_inf = 6000.0    -- m/s
...
129
```

- ▶ Reactions and energy exchange models from Kim and Jo, 2021
- ▶ Ionisation rates are based on the classic Park, 1993 model
- ▶ Includes chemical/exchange coupling from Knab, Fruhauf, and Messerschmid, 1995

Example Script: Inflow Conditions

```
18 nsp, nmodes, gmodel = setGasModel('gm-air11-2T.lua')
19 config.reactng = true
20 config.reactions_file = 'rr-kim-air11-2T.lua'
21 config.energy_exchange_file = 'ee-kim-air11-2T.lua'
22
23 T_inf = 270.65      -- K
24 rho_inf = 0.000977521752421559  -- kg/m^3
25 mass_fraction = {N2=0.767, O2=0.233}
26 u_inf = 6000.0    -- m/s
27
28 -- Compute full inflow state from T,rho, and u
29 Q = GasState:new{gmodel}
30 Q.T = T_inf;
31 Q.rho = rho_inf;
32 Q.massf = mass_fraction
33 Q.T_modes = {T_inf}
34 gmodel:updateThermoFromRHOT(Q);
35 p_inf = Q.p
36 inflow = FlowState:new{p=p_inf, T=T_inf, velx=u_inf, vely=0.0,
37                        massf=mass_fraction, T_modes={T_inf}}
38
39 initial=FlowSolution:new{jobName="etc",dir=" ../one",tindx=40,nBlocks=16}
...
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```

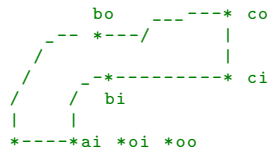
Example Script: Initial conditions

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23 T_inf = 270.65      -- K
24 rho_inf = 0.000977521752421559  -- kg/m^3
25 mass_fraction = {N2=0.767, O2=0.233}
26 u_inf = 6000.0     -- m/s
27
28 -- Compute full inflow state from T,rho, and u
29 Q = GasState:new{gmodel}
30 Q.T = T_inf;
31 Q.rho = rho_inf;
32 Q.massf = mass_fraction
33 Q.T_modes = {T_inf}
34 gmodel:updateThermoFromRHOT(Q);
35 p_inf = Q.p
36 inflow = FlowState:new{p=p_inf, T=T_inf, velx=u_inf, vely=0.0,
37                        massf=mass_fraction, T_modes={T_inf}}
38
39 initial=FlowSolution:new{jobName="etc",dir=" ../one",tindx=40,nBlocks=16}
40
41 -- Grid Geometry Specs --
42 ri = 0.010
43 thetai = math.rad(6.0)
44 ro = 0.015
45 diffo = 0.003
46 thetao = math.rad(30.0)
47 L = 0.0202+ri
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```

Example Script: Gridding

```
39  initial=FlowSolution:new{jobName="etc",dir="../one",tindx=40,nBlocks=16}
40
41  -- Grid Geometry Specs  --
42  ri = 0.010
43  thetai = math.rad(6.0)
44  ro = 0.015
45  diffo = 0.003
46  thetao = math.rad(30.0)
47  L = 0.0202+ri
48
49  oi = Vector3:new{x=ri, y=0.0}
50  ai = oi + ri*Vector3:new{x=-1.0, y=0.0}
51  bi = oi + ri*Vector3:new{x=-math.sin(thetai), y=math.cos(thetai)}
52  dxci = L - bi.x
53  dyci = dxci*math.tan(thetai)
54  ci = Vector3:new{x=bi.x + dxci, y=bi.y+dyci}
55  aibi = Arc:new{p0=ai, p1=bi, centre=oi}
56  bici = Line:new{p0=bi, p1=ci}
57  aici = Polyline:new{segments={aibi, bici}}
58
59  aoco = Spline2:new{filename="../one/shock_shape.dat"}
...
129
```



Example Script: More Gridding

```
49 oi = Vector3:new{x=ri, y=0.0}
50 ai = oi + ri*Vector3:new{x=-1.0, y=0.0}
51 bi = oi + ri*Vector3:new{x=-math.sin(thetai), y=math.cos(thetai)}
52 dxci = L - bi.x
53 dyci = dxci*math.tan(thetai)
54 ci = Vector3:new{x=bi.x + dxci, y=bi.y+dyci}
55 aibi = Arc:new{p0=ai, p1=bi, centre=oi}
56 bici = Line:new{p0=bi, p1=ci}
57 aici = Polyline:new{segments={aibi, bici}}
58
59 aoco = Spline2:new{filename="../one/shock_shape.dat"}
...
74
75 grid = StructuredGrid:new{psurface=surface, niv=niv, njv=njv, cfList=cluster}
76
77 blocks = FBArray:new{grid=grid,
78                       initialState=initial,
79                       bcList={
80                           north=OutFlowBC_Simple:new{},
81                           west=InFlowBC_Supersonic:new{flowState=inflow},
82                           east=WallBC_NoSlip_FixedT:new{Twall=2000.0, group=1},
83                           nib=2, njb=8}
84
...
129
```

Example Script: Blocks and Boundary Conditions

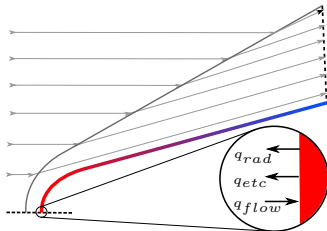
```
59 aoco = Spline2:new{filename="../one/shock_shape.dat"}
...
75 grid = StructuredGrid:new{psurface=surface, niv=niv, njv=njv, cfList=clusterlist}
76
77 blocks = FBArray:new{grid=grid,
78     initialState=initial,
79     bcList={
80         north=OutFlowBC_Simple:new{},
81         west=InFlowBC_Supersonic:new{flowState=inflow},
82         east=WallBC_ThermionicEmission:new{emissivity=0.89,
83             ThermionicEmissionActive=0,
84             group="wall"}},
85     nib=2, njb=8}
86
87 identifyBlockConnections()
88
89 config.write_loads = true
90 config.boundary_groups_for_loads = "wall"
...
129
```

$$0 = q_{flow} - q_{rad} - q_{etc} \quad (2)$$

$$q_{flow} = \kappa \frac{\partial T}{\partial x} - \sum_s h_s D_s \frac{\partial Y_s}{\partial x}$$

$$q_{rad} = \epsilon \sigma_S B T^4$$

$$q_{etc} = \frac{A_r T^2 \exp\left(\frac{-\Phi}{k_B T}\right)}{Q_e} (\Phi + 2k_B T)$$



Example Script: Loads Output Options

```
87 identifyBlockConnections()
88
89 config.write_loads = true
90 config.boundary_groups_for_loads = "wall"
91
92 SteadyStateSolver{
93     precondition_matrix_type = "ilu",
94     frozen_preconditioner_count = 100,
95     ...
129
```


Interlude: The Steady State Solver

- ▶ At each iteration the steady state solver solves a matrix problem:

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

- ▶ Most important takeaways:
 - ▶ The matrix is solved iteratively
 - ▶ The solution is built out of a linear combination of vectors
 - ▶ We use a preconditioner to make the matrix easier to solve

$$\mathbf{x}_n = \mathbf{x}_0 + Q_n \mathbf{y}_n$$

$$\begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_j \end{bmatrix} = \begin{bmatrix} Q_{00} \\ Q_{10} \\ \vdots \\ Q_{j0} \end{bmatrix} \begin{bmatrix} y_0 \end{bmatrix} \quad \rightarrow \quad \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_j \end{bmatrix} = \begin{bmatrix} Q_{00} & Q_{01} \\ Q_{10} & Q_{11} \\ \vdots & \vdots \\ Q_{j0} & Q_{j1} \end{bmatrix} \begin{bmatrix} y_0 \\ y_1 \end{bmatrix}$$

Example Script: Steady State Solver Preconditioner

```
89 config.write_loads = true
90 config.boundary_groups_for_loads = "wall"
91
92 SteadyStateSolver{
93     precondition_matrix_type = "ilu",
94     frozen_preconditioner_count = 100,
95
96     max_outer_iterations = 40,
97     max_restarts = 10,
98     use_complex_matvec_eval = true,
99     ...
129 }
```

Example Script: Newton-Krylov Configuration

```
92 SteadyStateSolver{
93     precondition_matrix_type = "ilu",
94     frozen_preconditioner_count = 100,
95
96     max_outer_iterations = 40,
97     max_restarts = 10,
98     use_complex_matvec_eval = true,
99
100    number_total_steps = 6000,
101    stop_on_relative_global_residual = 1e-6,
102    ...
129 }
```

$$= \begin{bmatrix} Q_{00} & Q_{01} & \dots & Q_{0,40} \\ Q_{10} & Q_{11} & \dots & Q_{1,40} \\ \vdots & \vdots & \dots & \vdots \\ Q_{j0} & Q_{j1} & \dots & Q_{j,40} \end{bmatrix}$$

Example Script: Stopping Criteria

```
96     max_outer_iterations = 40,
97     max_restarts = 10,
98     use_complex_matvec_eval = true,
99
100    number_total_steps = 6000,
101    stop_on_relative_global_residual = 1e-6,
102
103    residual_based_cfl_scheduling = false,
104    cfl_schedule_length = 12,
105    cfl_schedule_value_list = {
106        0.1, 0.2, 0.5, 1.0, 2.0, 5.0, 10.0, 20.0, 50.0, 80.0, 100.0, 200.0,
107    },
108    cfl_schedule_iter_list = {
109        1, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 1100
110    },
111    ...
129
```

Example Script: Timestep Scheduling

```
100     number_total_steps = 6000,  
101     stop_on_relative_global_residual = 1e-6,  
102  
103     residual_based_cfl_scheduling = false,  
104     cfl_schedule_length = 12,  
105     cfl_schedule_value_list = {  
106         0.1, 0.2, 0.5, 1.0, 2.0, 5.0, 10.0, 20.0, 50.0, 80.0, 100.0, 200.0  
107     },  
108     cfl_schedule_iter_list = {  
109         1, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 1100  
110     },  
111  
112     -- Settings for start-up phase  
113     number_start_up_steps = 0,  
114     cfl0 = 0.1,  
115     eta0 = 0.008,  
116     sigma0 = 1.0e-30,  
...  
129
```

Example Script: Start-up Phase Configuration

```
103     residual_based_cfl_scheduling = false,
104     cfl_schedule_length = 12,
105     cfl_schedule_value_list = {
106         0.1, 0.2, 0.5, 1.0, 2.0, 5.0, 10.0, 20.0, 50.0, 80.0, 100.0, 200.0,
107     },
108     cfl_schedule_iter_list = {
109         1, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 1100
110     },
111
112     -- Settings for start-up phase
113     number_start_up_steps = 0,
114     cfl0 = 0.1,
115     eta0 = 0.008,
116     sigma0 = 1.0e-30,
117
118     -- Settings for main solution phase
119     cfl1 = 0.1,
120     eta1 = 0.001,
121     sigma1 = 1.0e-30,
122     eta_strategy = "constant",
123     ...
129
```

Example Script: Main Phase Configuration

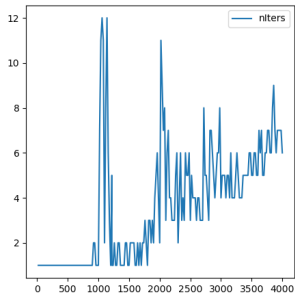
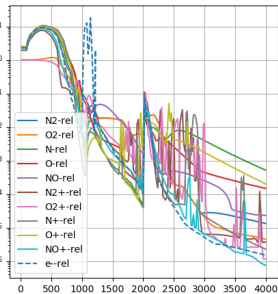
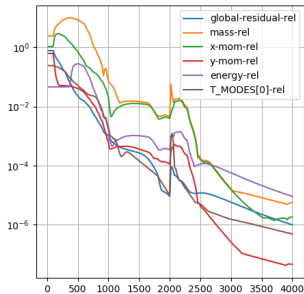
```
112 -- Settings for start-up phase
113 number_start_up_steps = 0,
114 cfl0 = 0.1,
115 eta0 = 0.008,
116 sigma0 = 1.0e-30,
117
118 -- Settings for main solution phase
119 cfl1 = 0.1,
120 eta1 = 0.001,
121 sigma1 = 1.0e-30,
122 eta_strategy = "constant",
123
124 -- Settings control write-out
125 snapshots_count = 100,
126 number_total_snapshots = 1000,
127 write_diagnostics_count = 20,
128 write_loads_count = 100,
129 }
```

$$\mathbf{x}_n = \mathbf{x}_0 + Q_n \mathbf{y}_n$$

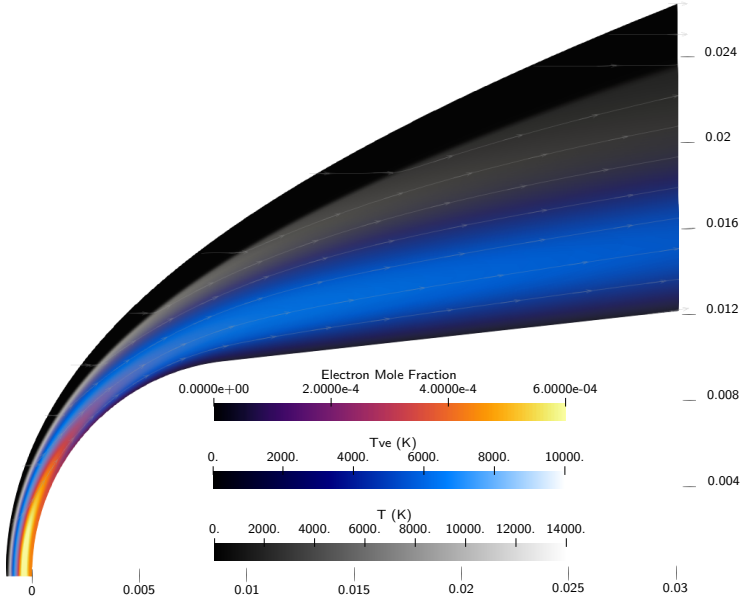
Example Script: Output Configuration

```
118     -- Settings for main solution phase
119     cfl1 = 0.1,
120     eta1 = 0.001,
121     sigma1 = 1.0e-30,
122     eta_strategy = "constant",
123
124     -- Settings control write-out
125     snapshots_count = 100,
126     number_total_snapshots = 1000,
127     write_diagnostics_count = 20,
128     write_loads_count = 100,
129 }
```

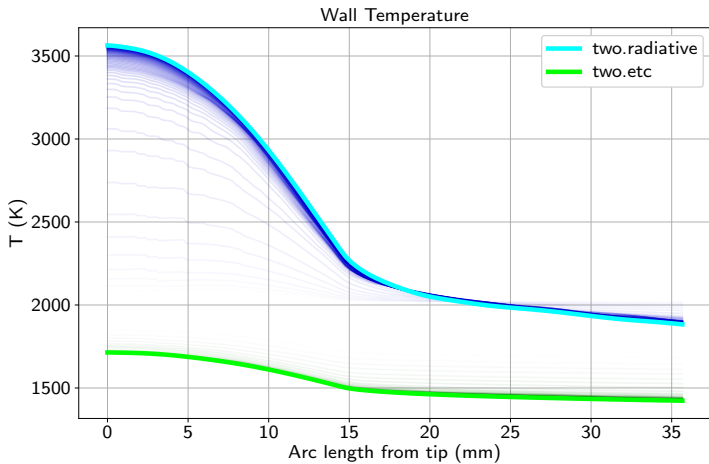

Results: Residual Drop



Results: Flow Solution



Results: Wall Temperature



Thanks for listening!

References:

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