German Research School
for Simulation Sciences

Unstructured Finite Element Solver (ft. FEniCS)

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SiSc. Lab Presentation

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Contents

Motivation

$$\frac{\partial T}{\partial t} - \alpha \nabla^2 T = 0 \quad in \;\; \Omega \tag{1}$$

$$\begin{aligned} T &= T_D \quad on \;\; \Gamma_D \\ -k\nabla T &= q \quad\;\; on \;\; \Gamma_N \end{aligned} \tag{2}$$

$$\alpha = \frac{k}{c_p \rho} \tag{3}$$

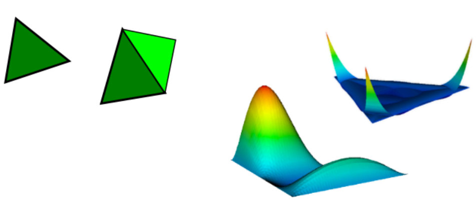
$$\frac{\partial T}{\partial t} = \frac{T^{n+1} - T^n}{\Delta t} + O(\Delta t) \tag{4}$$

$$T^{n+1} = T^n + \Delta t(\alpha \nabla^2 T) \tag{5}$$

$$\begin{aligned} S :&= \{T \in H^1(\Omega) \mid T = T_D \quad on \;\; \Gamma_D\} \\ V :&= \{w \in H^1(\Omega) \mid w = 0 \quad\;\; on \;\; \Gamma_D\} \end{aligned} \tag{6}$$

$$\int_\Omega w T^{n+1} d\Omega - \int_\Omega w T^n d\Omega + \int_\Omega \Delta t(\alpha \nabla w \cdot \nabla T^{n+1}) d\Omega - \int_{\Gamma_N} \Delta t(\alpha \frac{q}{k}) w \hat{n} \cdot d\Gamma \tag{7}$$

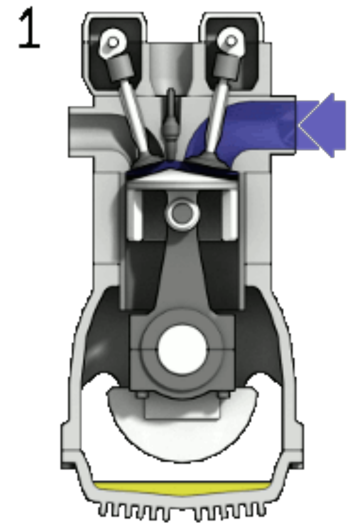
$\mathcal{T}$ $\qquad$ $\mathcal{V}$ $\qquad$ $\mathcal{L}$

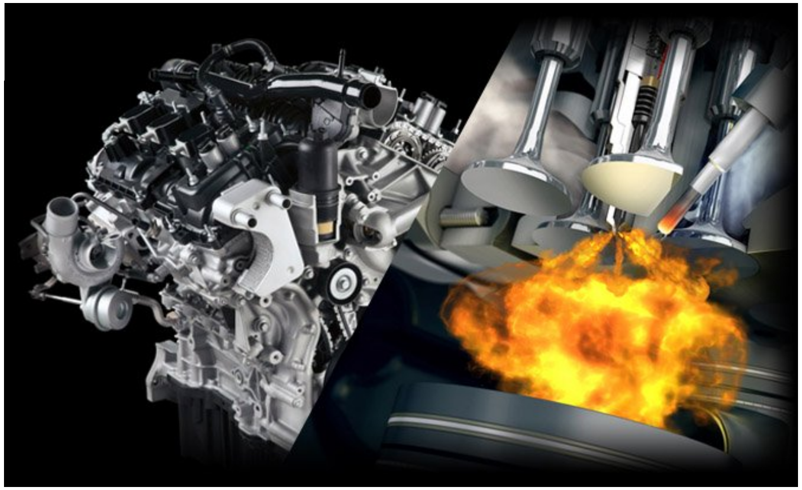


$v(\bar{x})$

$v(\bar{x}) \cdot n$

$\int_T v(x) w(x) \, \mathrm{d}x$





Setup and workflow

Docker
Community Edition

Version 18.03.1-ce-win65 (17513)
Channel: stable
93354b3

CONDA®

Preprocessing → Processing → Postprocessing

gmsh

FEniCS PROJECT

ParaView

Main options for visualisation
- Built-in VTK plotting
- Matplotlib
- ParaView

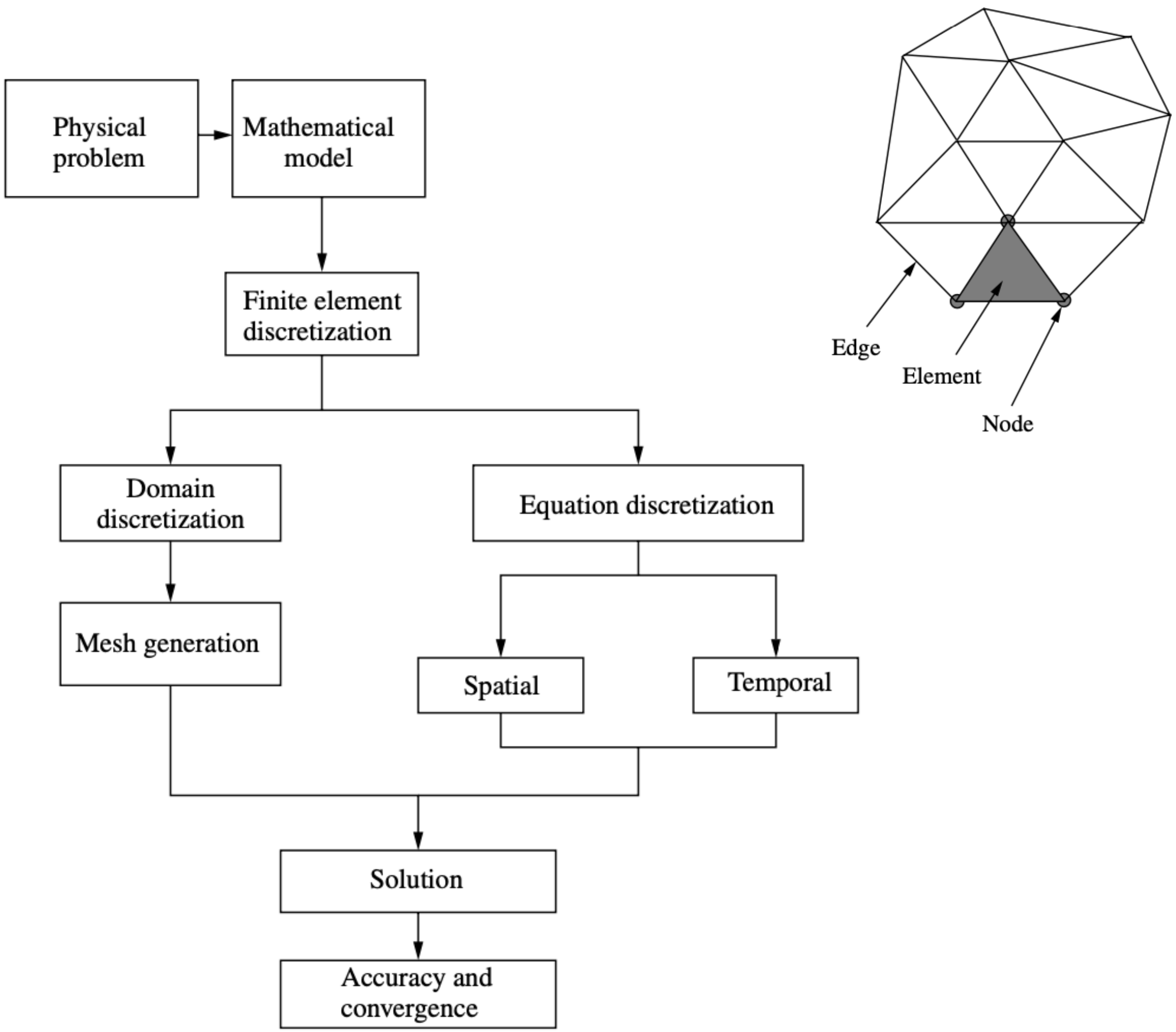
Introducing… FEniCS

- Automated programming environment for differential equations
  - C++/Python library
  - Initiated 2003 in Chicago
  - 1000–2000 monthly downloads
  - Part of Debian and Ubuntu
  - Licensed under the GNU LGPL

- Automated FEM

`http://fenicsproject.org/`

Mathematical background



(a) Numerical model for heat transfer calculations

Mathematical background

$$\frac{\partial T}{\partial t} - \alpha \nabla^2 T = 0 \quad in \;\; \Omega \tag{1}$$

$$\begin{aligned} T &= T_D \quad && on \;\; \Gamma_D \\ -k\nabla T &= q && on \;\; \Gamma_N \end{aligned} \tag{2}$$

$$\alpha = \frac{k}{c_p \rho} \tag{3}$$

$$\frac{\partial T}{\partial t} = \frac{T^{n+1} - T^n}{\Delta t} + O(\Delta t) \tag{4}$$

$$T^{n+1} = T^n + \Delta t (\alpha \nabla^2 T) \tag{5}$$

$$\begin{aligned} S &:= \{T \in H^1(\Omega) \mid T = T_D \quad on \;\; \Gamma_D\} \\ V &:= \{w \in H^1(\Omega) \mid w = 0 \qquad on \;\; \Gamma_D\} \end{aligned} \tag{6}$$

$$\int_\Omega w\, T^{n+1} d\Omega - \int_\Omega w T^n d\Omega + \int_\Omega \Delta t\, (\alpha \nabla w . \nabla T^{n+1}) d\Omega - \int_{\Gamma_n} \Delta t \frac{\alpha}{k} (\hat{n}.\vec{q})\; w\; d\Gamma = 0 \tag{7}$$

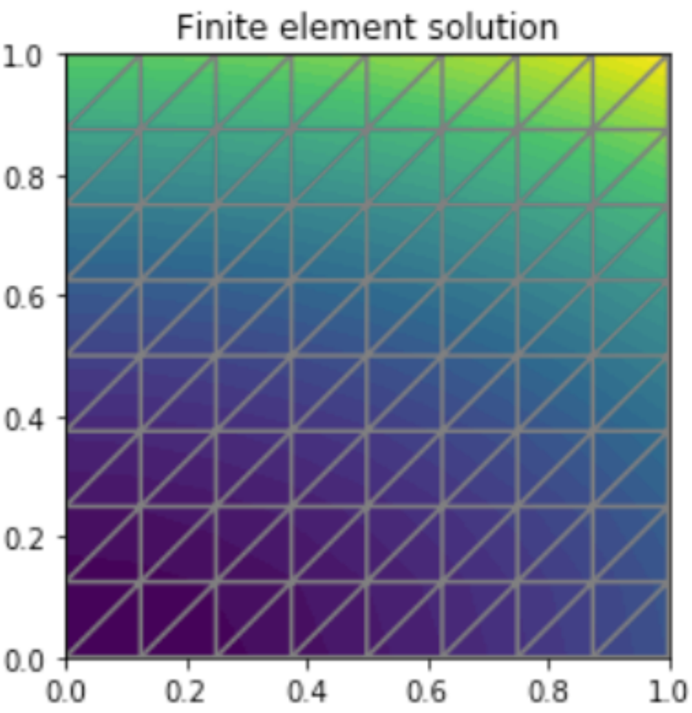
Case 1 – 2D Heat Equation – Demo

[demo_fenics_2dsquare.ipynb]

$$
\begin{aligned}
\frac{\partial u}{\partial t} &= \nabla^2 u + f && \text{in } \Omega \times (0, T], \\
u &= u_{\mathrm{D}} && \text{on } \partial\Omega \times (0, T], \\
u &= u_0 && \text{at } t = 0 .
\end{aligned}
$$

Validation:

$$u = 1 + x^2 + \alpha y^2 + \beta t,$$



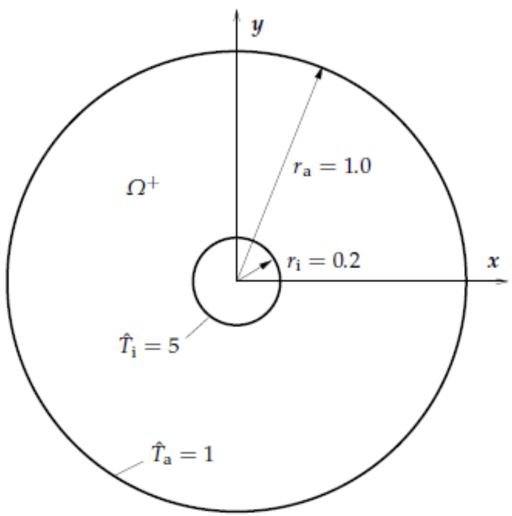
(a) Solution and mesh

Case 2 – 2D Cylinder – Problem description

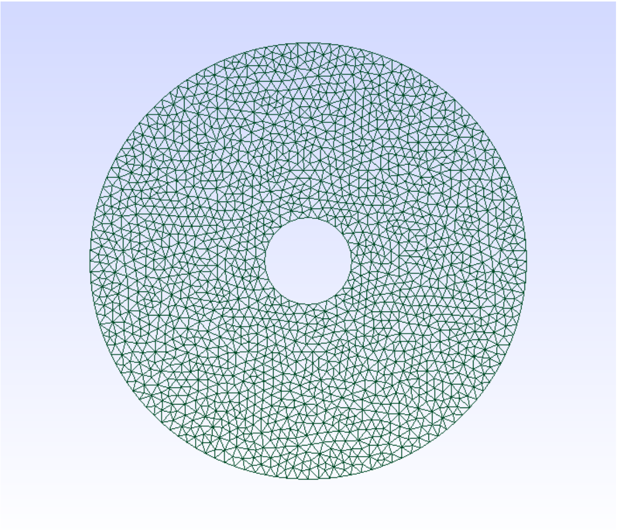
- **PDE:** Time-dependent Heat(Diffusion) Equation
- **Boundary Condition:** Dirichlet
- **Time Domain:** Steady
- **Validation:**

$$
\begin{aligned}
u_t &= \kappa * \Delta u + f \\
u &= T_i \quad \textit{on inner cylinder} \\
u &= T_a \quad \textit{on outer cylinder} \\
f &= 0
\end{aligned}
$$

$$T_{cyl}^{exact}\big(r(x)\big) = T_i - (\ln(r) - \ln(r_a))\frac{T_i - T_a}{\ln(r_a) - \ln(r_i)}$$ (Analytical solution) [1]



(a) 2D Setup



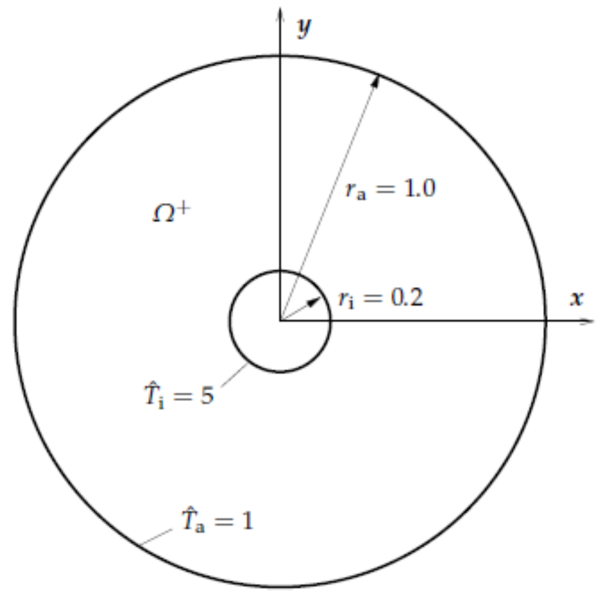
(b) Meshed Domain

Mesh details:
Refinement level (h) = 0.05 m
No. of elements = 3572
No. of nodes = 1864

Case 2 – 2D Cylinder – Setup

- Boundary conditions:

Boundary ID	Comment	Type	Value	Unit
T_a	Outer	Dirichlet	1	°C
T_i	Inner	Dirichlet	5	°C

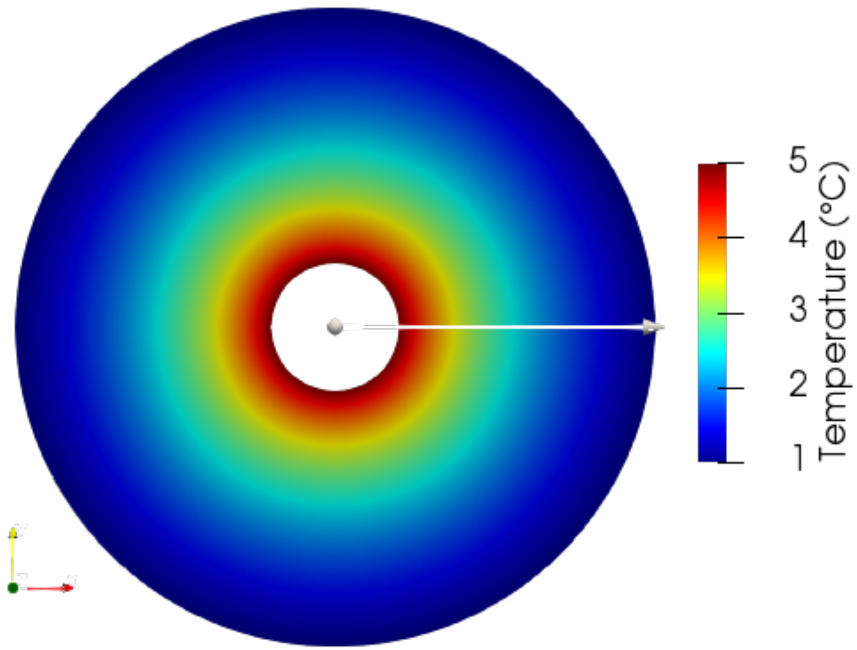


(c) Boundary conditions

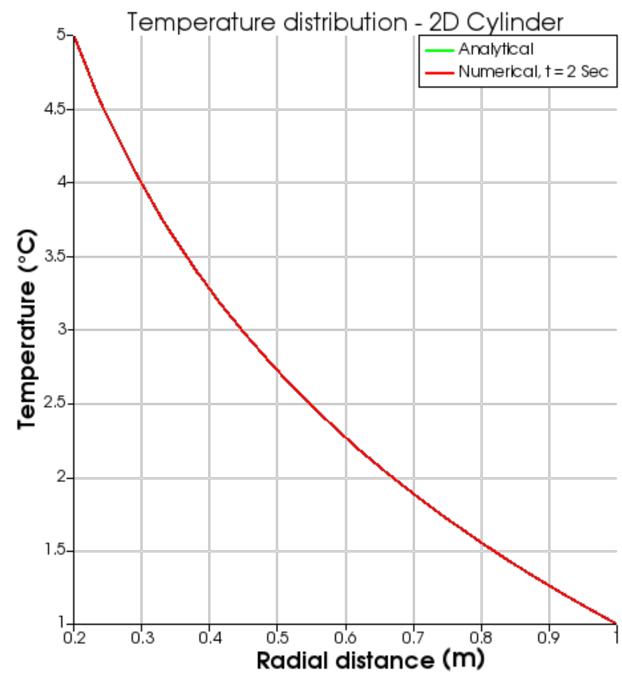
- Weak form:

$$\int_{\Omega} w\, T^{n+1} d\Omega - \int_{\Omega} w T^{n} d\Omega + \int_{\Omega} \Delta t\, (\alpha \nabla w . \nabla T^{n+1}) d\Omega - \int_{\Gamma_n} \Delta t \cancelto{= 0}{\frac{\alpha}{k} (\vec{n} . \vec{q})}\, w\, d\Gamma = 0$$

Case 2 – 2D Cylinder – Results

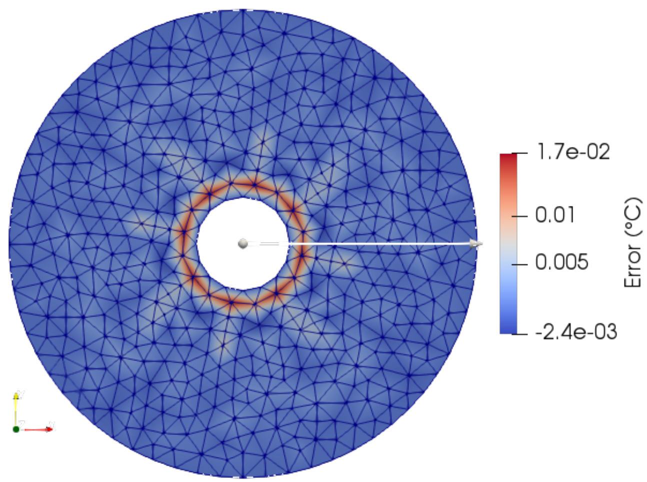


(d) Contour plot

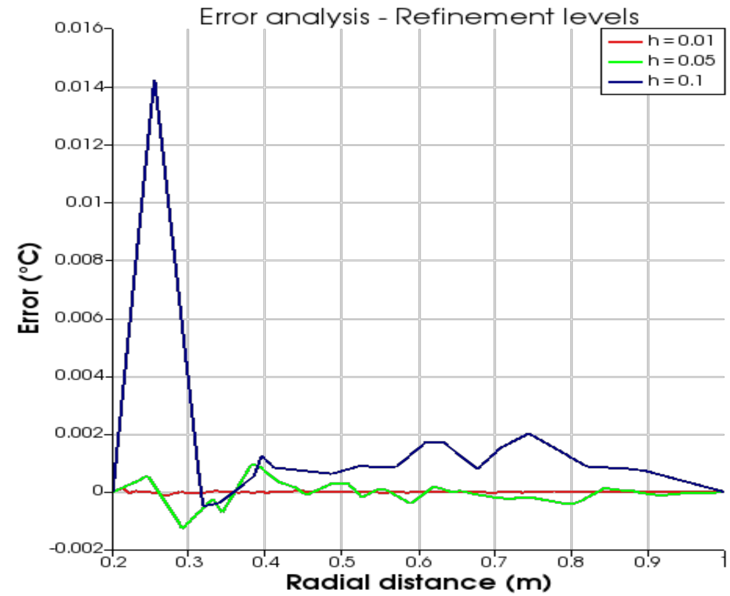


(e) Line plot

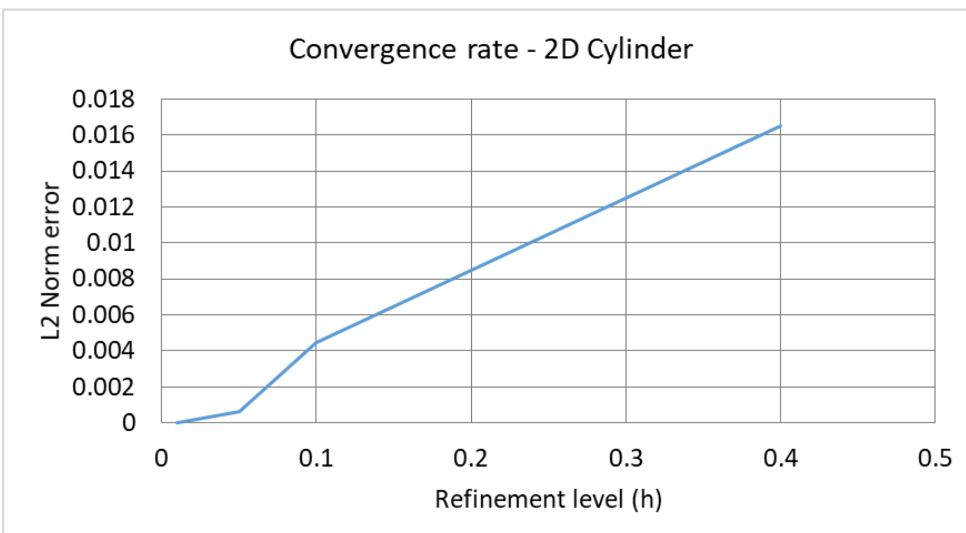
Case 2 – 2D Cylinder – Error analysis



(f) Error contour (h = 0.1 m)



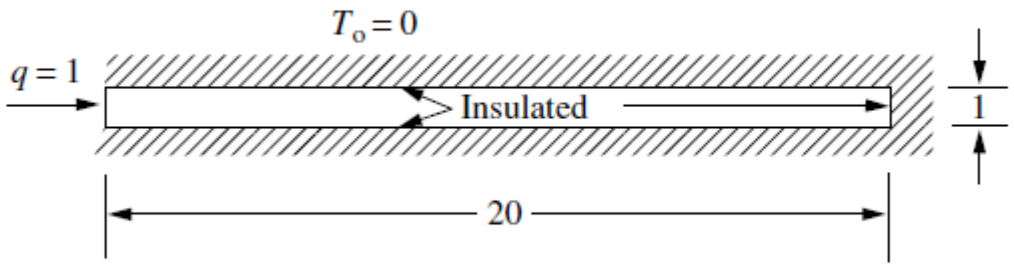
(g) Error line plot



Case 3 – 2D Rod – Problem description

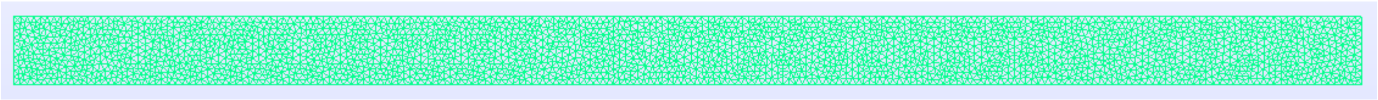
- **PDE:** Time-dependent Heat(Diffusion) Equation
- **Boundary Condition:** Neumann
- **Time Domain:** Unsteady (Transient)
- **Validation:**

$$T(x,t) = 2(t/\pi)^{1/2}\left[\exp\left(-x^2/4t\right) - (1/2)x\sqrt{\frac{\pi}{t}}\,erfc\left(\frac{x}{2\sqrt{t}}\right)\right]$$ Analytical solution



(a) 2D setup

Mesh details:
Refinement level (h) = 0.1 m
No. of elements = 5220
No. of nodes = 2821

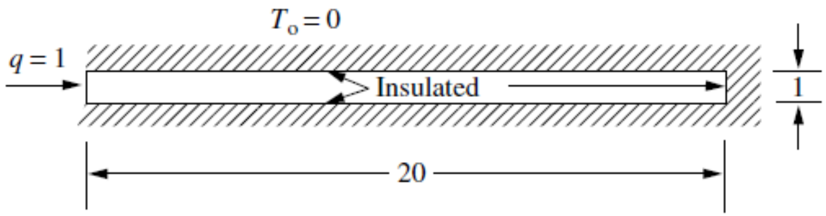


(b) Meshed domain

Case 3 – 2D Rod – Setup

- Boundary conditions:

Boundary ID	**Comment**	**Type**	**Value**	**Unit**
T_o	Insulated	Dirichlet	0	°C
q	Heat flux	Neumann	1	W/m²

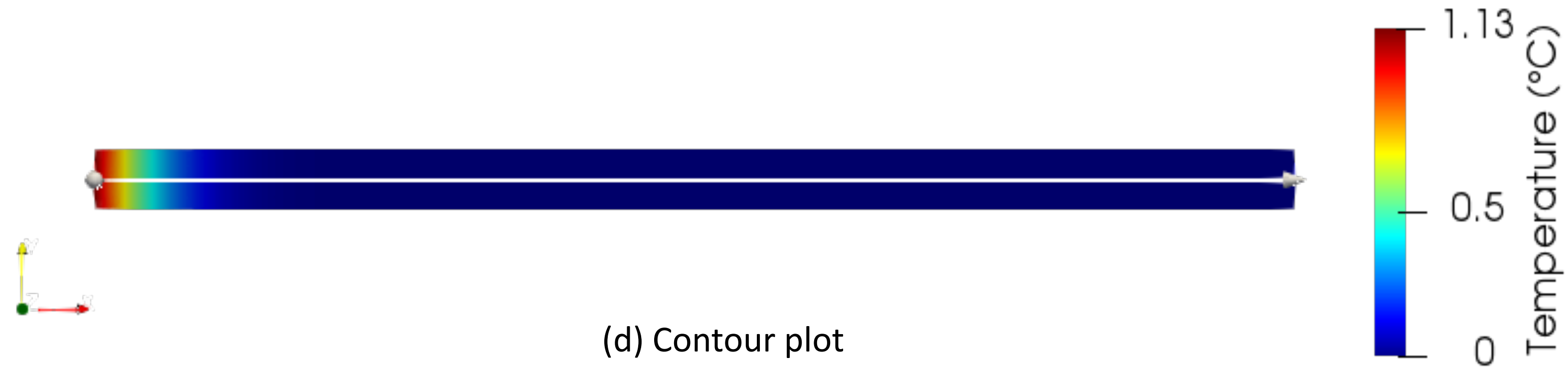


(c) Boundary conditions

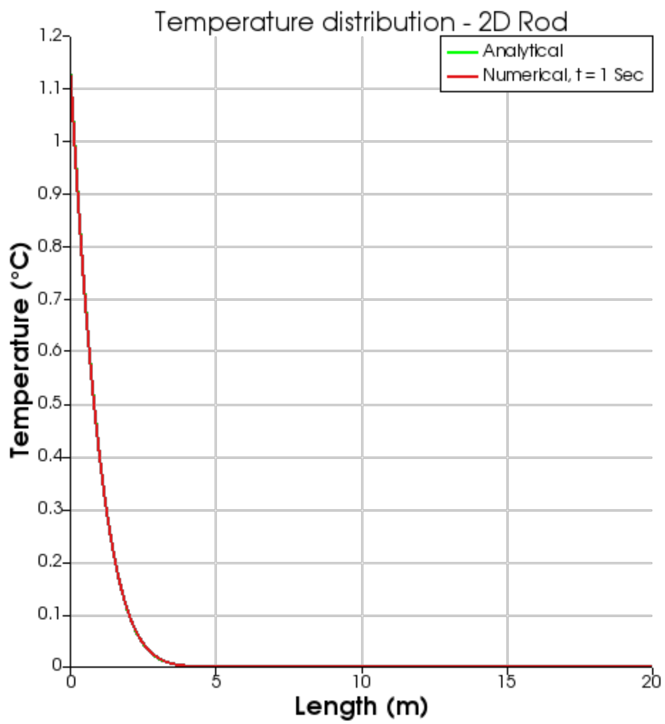
- Weak form:

$$\int_{\Omega} w\, T^{n+1} d\Omega - \int_{\Omega} w T^{n} d\Omega + \int_{\Omega} \Delta t\, (\alpha \nabla w . \nabla T^{n+1}) d\Omega - \boxed{\int_{\Gamma_n} \Delta t \frac{\alpha}{k} (\hat{n}.\vec{q})\; w\, d\Gamma} = 0$$

Case 3 – 2D Rod – Results

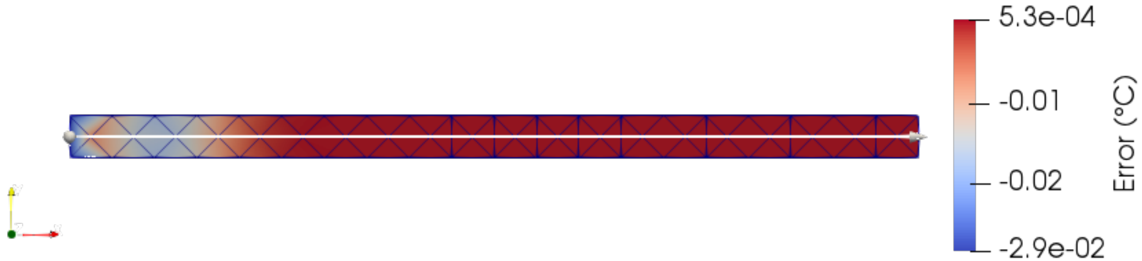


(d) Contour plot

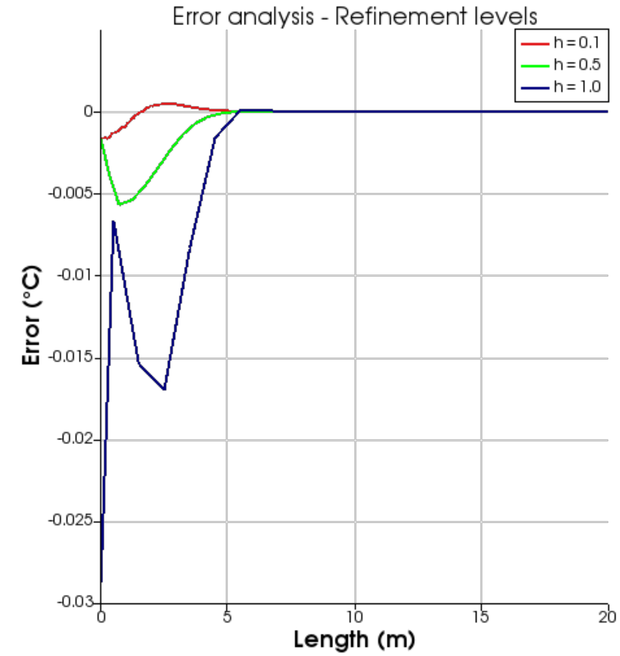


(e) Line plot

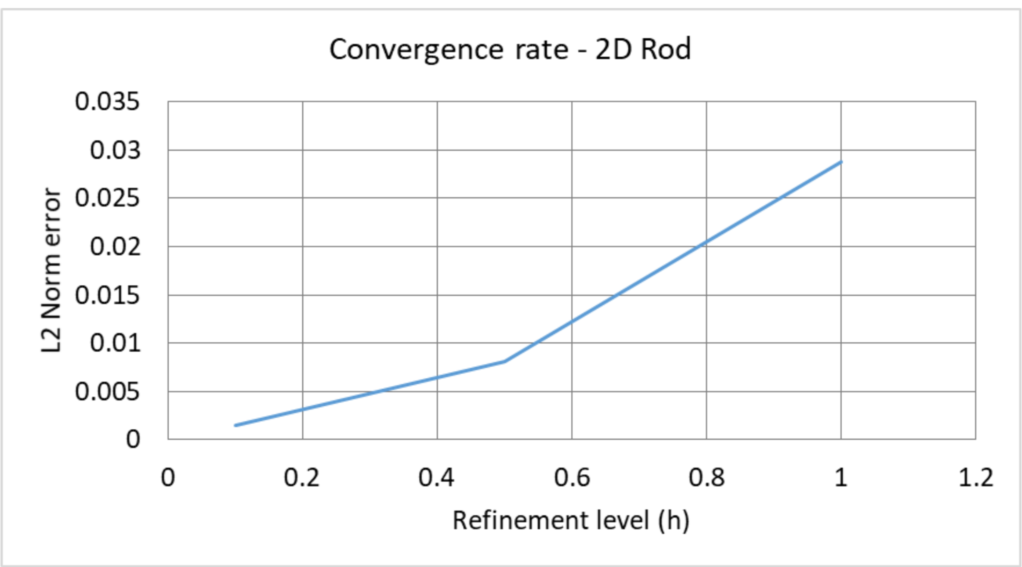
Case 3 – 2D Rod – Error analysis



(f) Error contour (h = 1.0 m)



(g) Error line plot



Real life application

Motivation

$$\frac{\partial T}{\partial t} - \alpha \nabla^2 T = 0 \quad in \ \Omega \tag{1}$$

$$\begin{aligned} T &= T_D \quad on \ \Gamma_D \\ -k\nabla T &= q \quad \ \ on \ \Gamma_N \end{aligned} \tag{2}$$

$$\alpha = \frac{k}{c_p \rho} \tag{3}$$

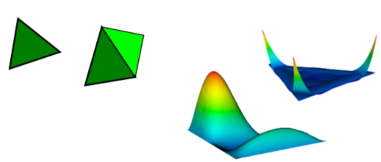
$$\frac{\partial T}{\partial t} = \frac{T^{n+1} - T^n}{\Delta t} + O(\Delta t) \tag{4}$$

$$T^{n+1} = T^n + \Delta t(\alpha \nabla^2 T) \tag{5}$$

$$\begin{aligned} S &:= \{T \in H^1(\Omega) \mid T = T_D \quad on \ \Gamma_D\} \\ V &:= \{w \in H^1(\Omega) \mid w = 0 \quad \ \ on \ \Gamma_D\} \end{aligned} \tag{6}$$

$$\int_\Omega w T^{n+1} d\Omega - \int_\Omega w T^n d\Omega + \int_\Omega \Delta t(\alpha \nabla w \cdot \nabla T^{n+1}) d\Omega - \int_{\Gamma_N} \Delta t(\alpha \frac{q}{k}) w \hat{n} \cdot d\Gamma \tag{7}$$

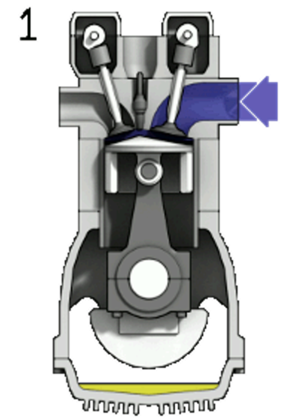
T $\mathcal{V}$ $\mathcal{L}$

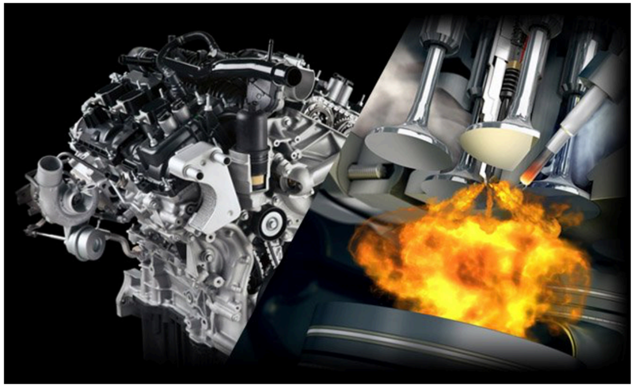


$v(\bar{x})$

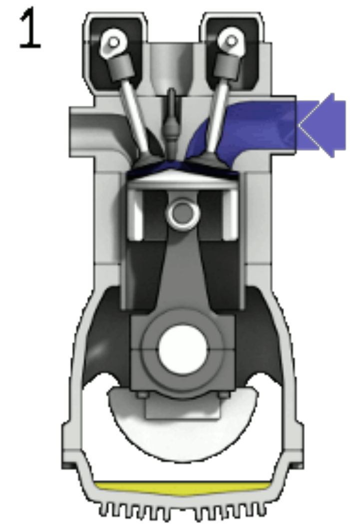
$v(\bar{x}) \cdot n$

$\int_T v(x) w(x) \, \mathrm{d}x$





Case 4 – 2D and 3D Piston

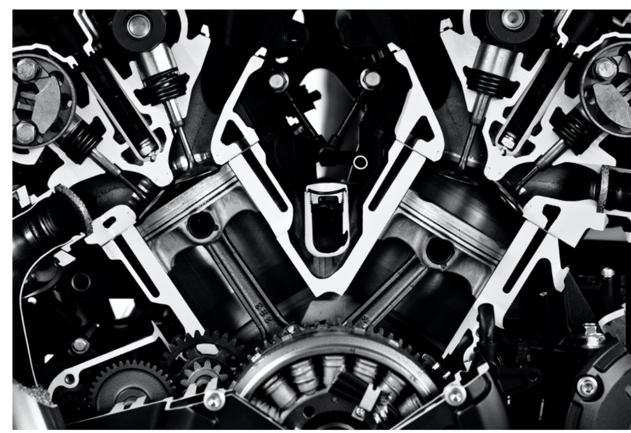


Motivation

- Reciprocating Piston
- Design for Durability and Performance
- Evaluate Cooling Performance

Material properties

- Material: Aluminum Alloy
- Thermal Diffusivity: $5.4 \times 10-5\ m^2/s$.



Case 4 – 2D and 3D Piston

- Subcase 1: Dirichlet

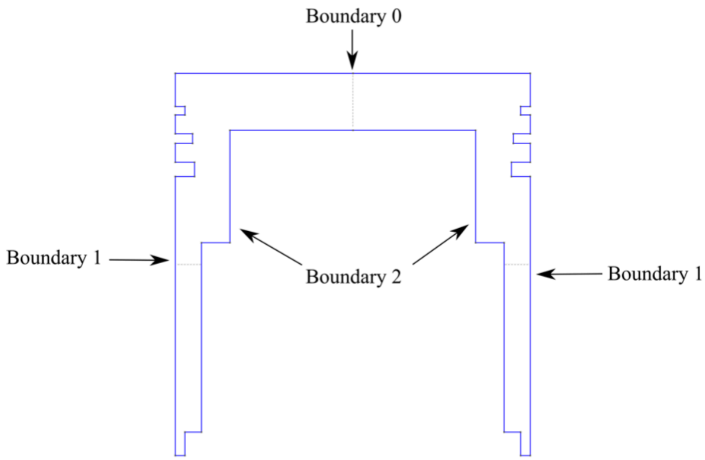
Boundary ID	Comment	Type	Value	Unit
0	Top	Dirichlet	300	°C
1	Liner	Dirichlet	100	°C
2	Piston underneath	Dirichlet	30	°C
3 (for 3D)	Symmetry plane	Neumann	0	$W \cdot m^{-2}$

- Subcase 2: Dirichlet and Neumann

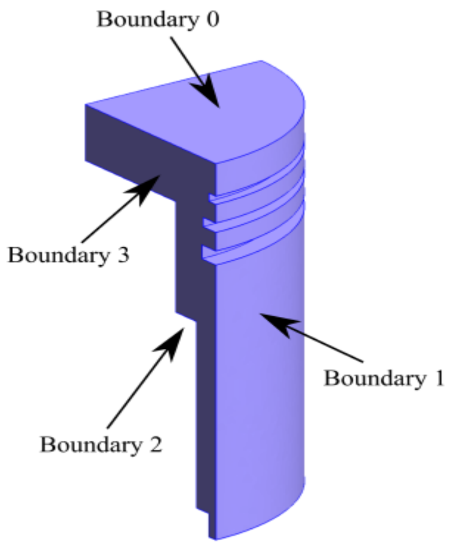
Boundary ID	Comment	Type	Value	Unit
0	Top	Neumann	2	$MW \cdot m^{-2}$
1	Liner	Dirichlet	100	°C
2	Piston underneath	Dirichlet	30	°C
3 (for 3D)	Symmetry plane	Neumann	0	$W \cdot m^{-2}$

- Subcase 3: Time-dependent Neumann

Boundary ID	Comment	Type	Value	Unit
0	Top	Neumann	q_dot	$MW \cdot m^{-2}$
1	Liner	Dirichlet	100	°C
2	Piston underneath	Dirichlet	30	°C
3 (for 3D)	Symmetry plane	Neumann	0	$W \cdot m^{-2}$



(a) Piston 2D setup

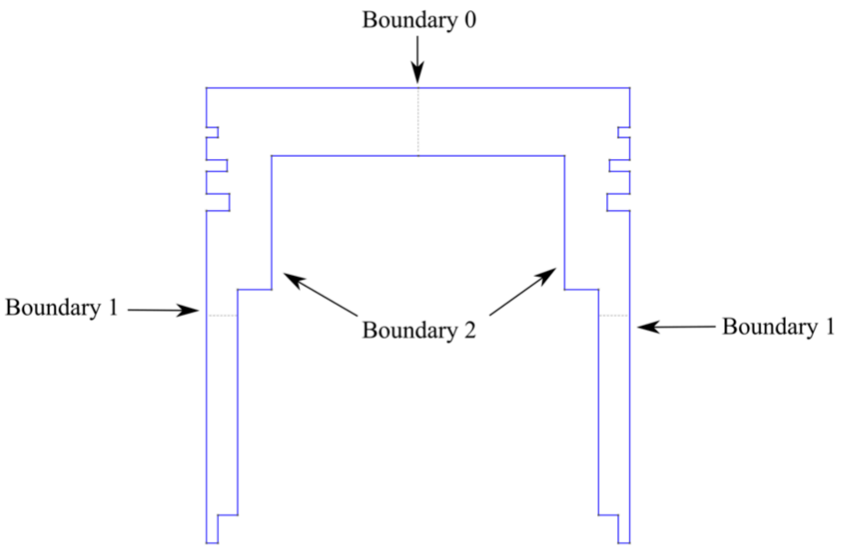


(b) Piston 3D setup

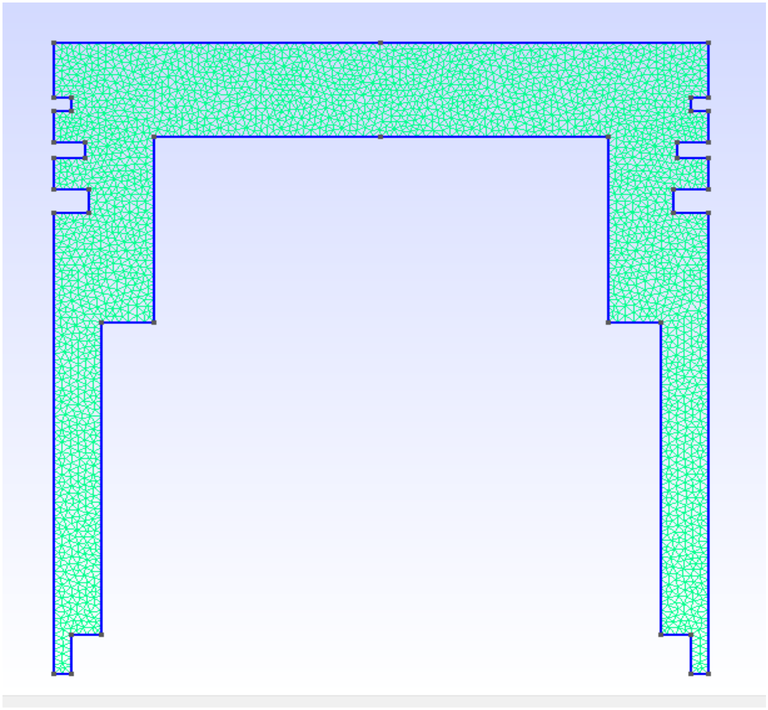
Case 4 – 2D Piston – Problem description

- **PDE:** Time-dependent Heat(Diffusion) Equation
- **Time Domain:** Unsteady (Transient)

Mesh details:
Refinement level (h) = 1 mm
No. of elements = 2810
No. of nodes = 5126



(a) 2D setup

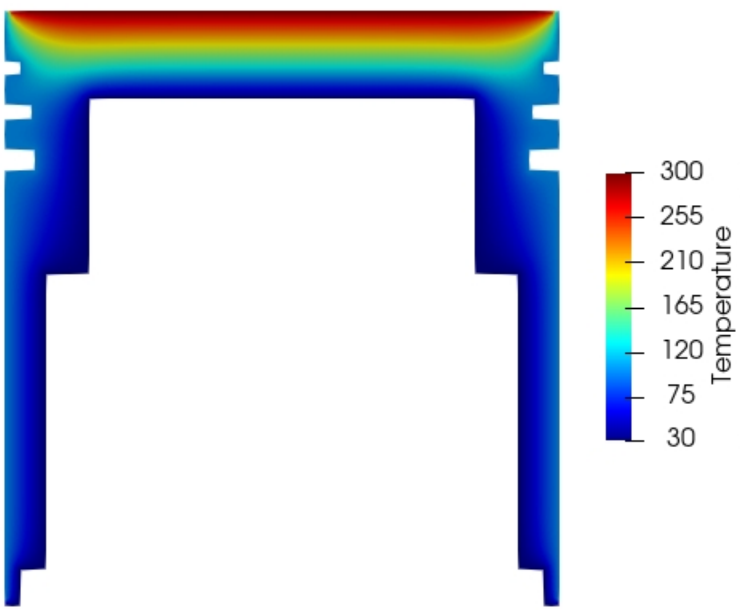


(b) Meshed domain

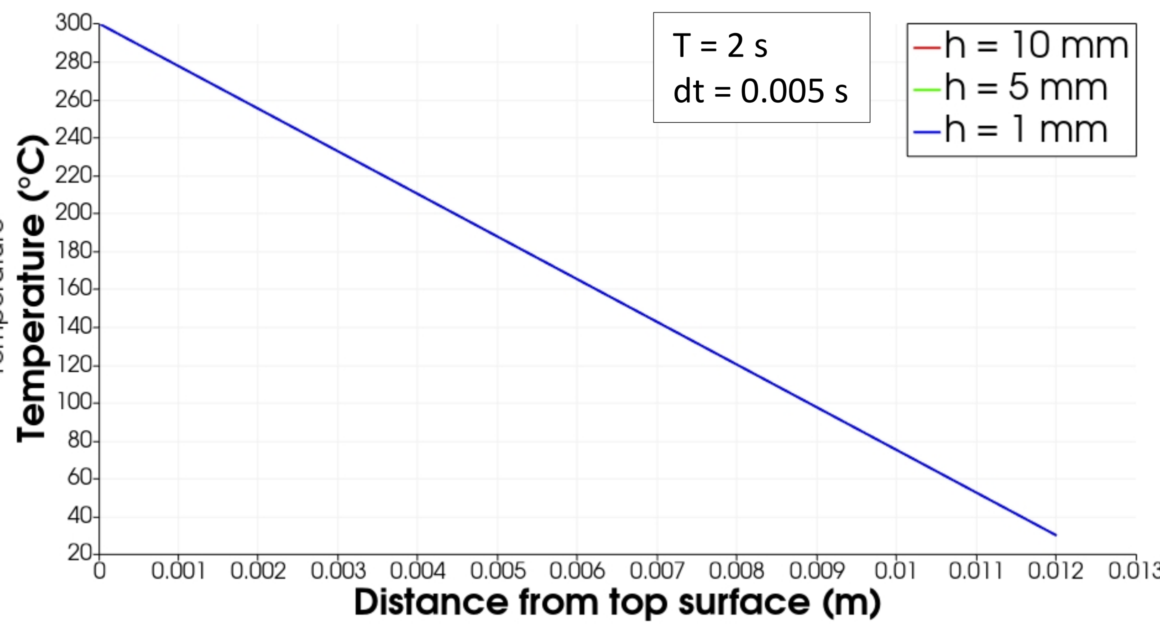
Case 4.1 – 2D Piston

- Subcase 1: Dirichlet BC

Boundary ID	Comment	Type	Value	Unit
0	Top	Dirichlet	300	°C
1	Liner	Dirichlet	100	°C
2	Piston underneath	Dirichlet	30	°C

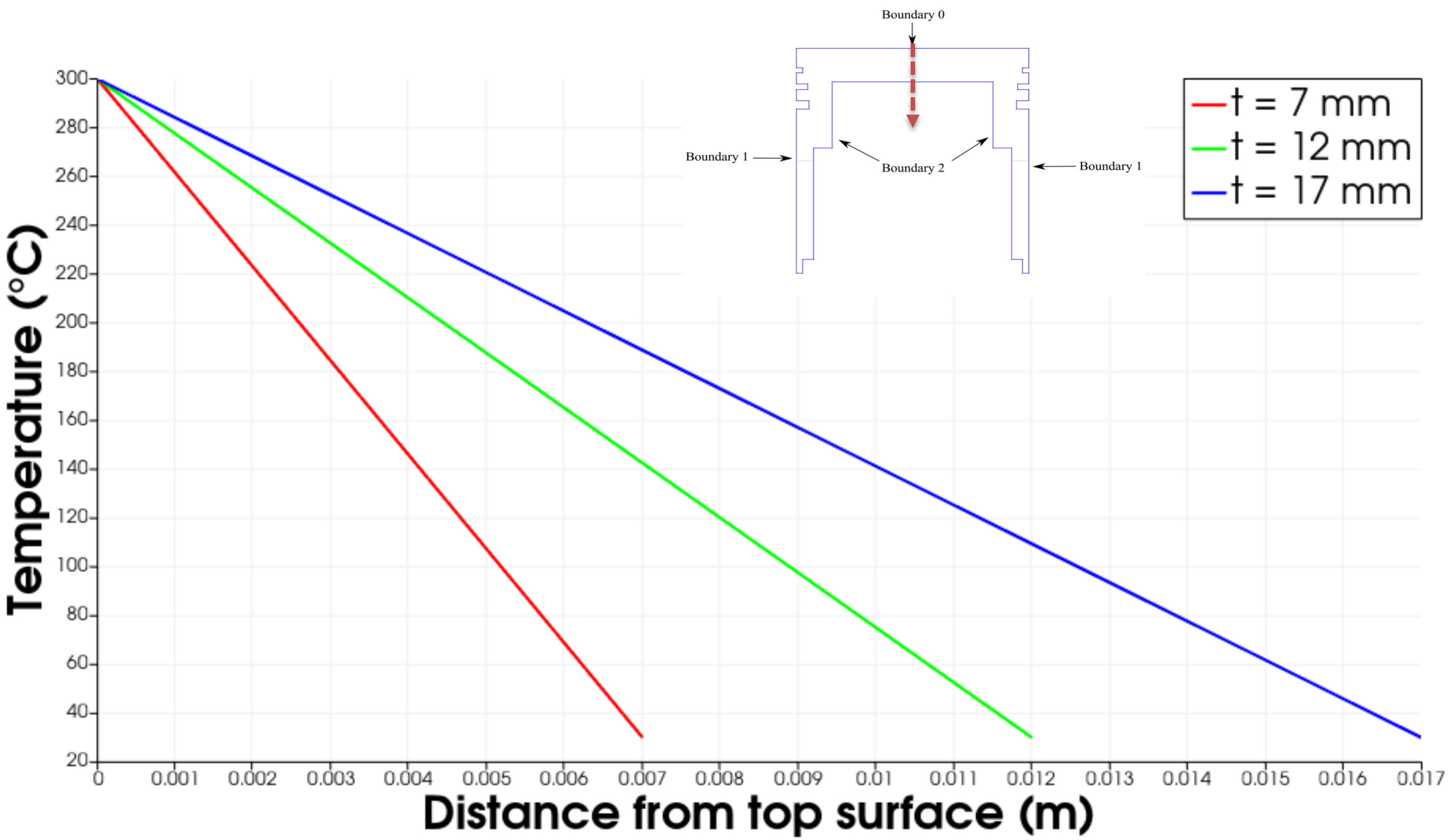


(a) Contour plot (h = 1mm)



(b) Mesh convergence study

Case 4.1 – 2D Piston – Thickness study

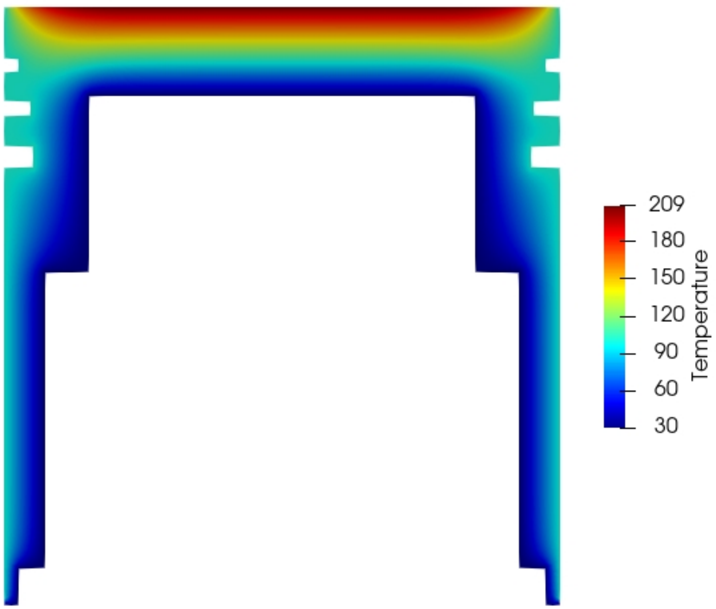


(c) Temperature distribution

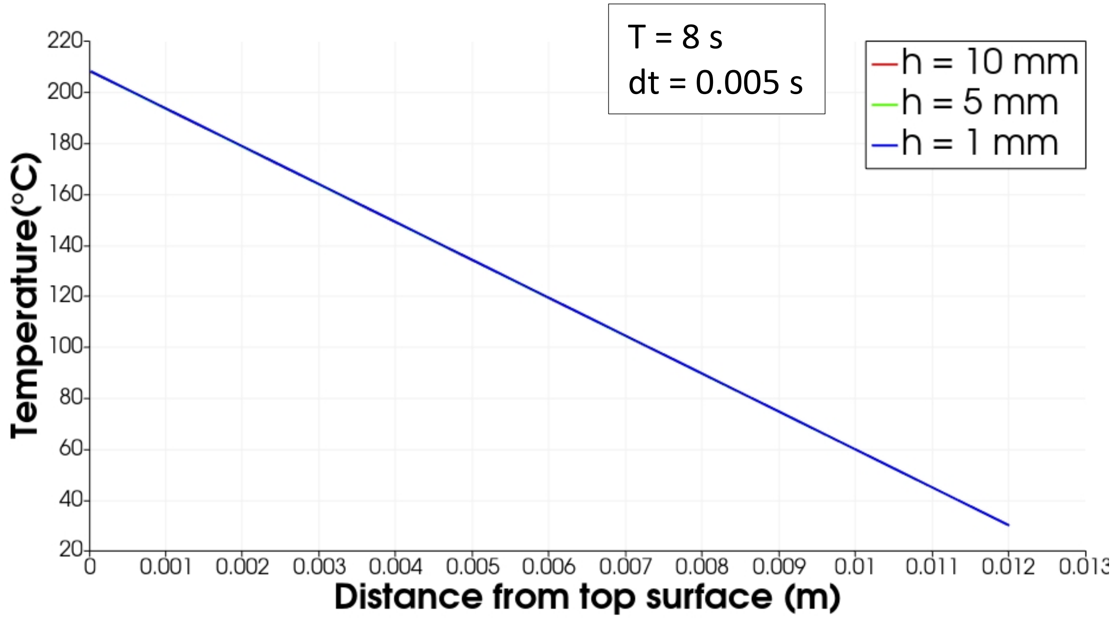
Case 4.2 – 2D Piston

- Subcase 2: Dirichlet and Neumann BC

Boundary ID	Comment	Type	Value	Unit
0	Top	Neumann	2	$MW \cdot m^{-2}$
1	Liner	Dirichlet	100	°C
2	Piston underneath	Dirichlet	30	°C

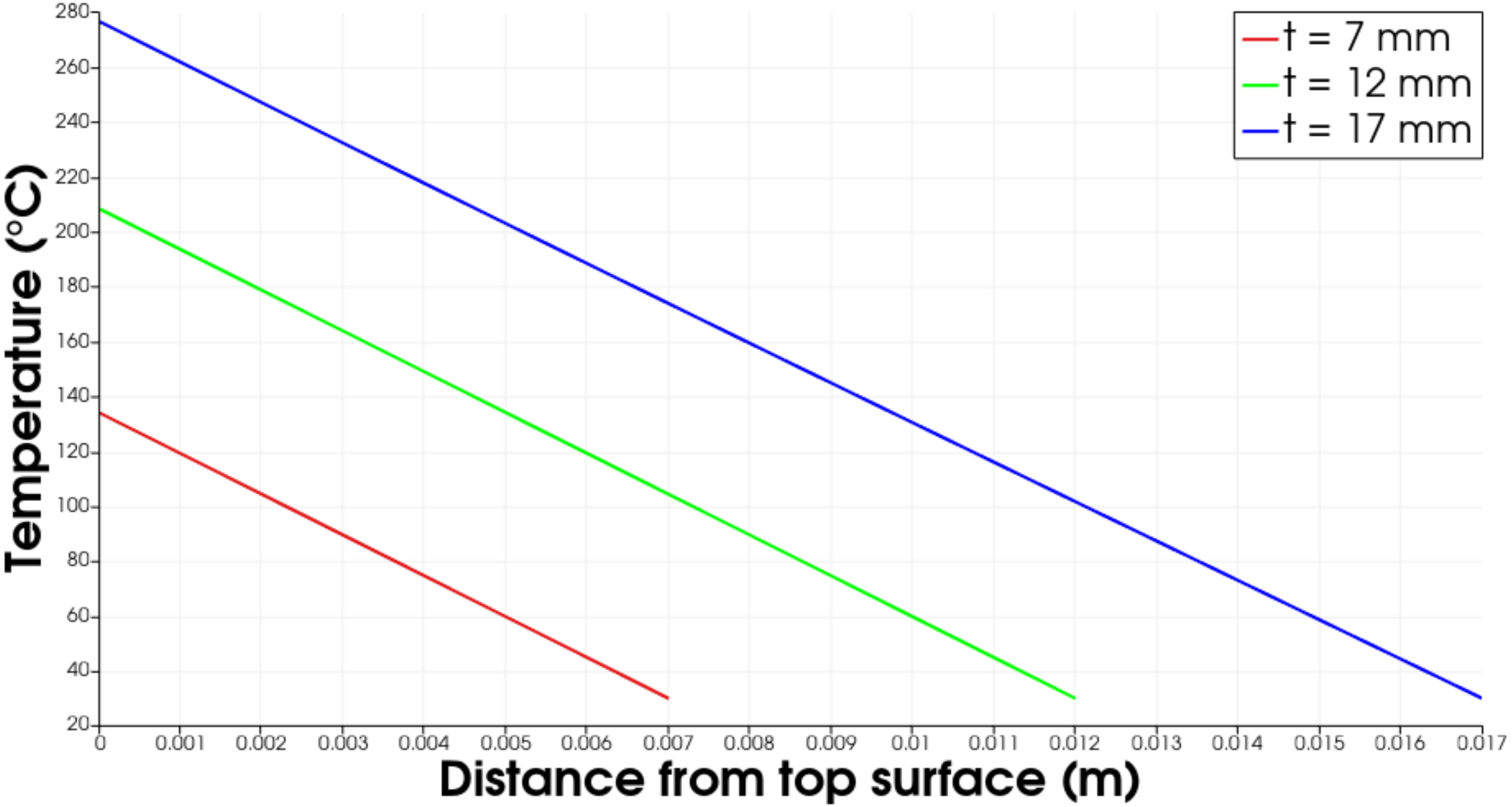


(a) Contour plot (h = 1mm)



(b) Mesh convergence study

Case 4.2 – 2D Piston – Thickness study



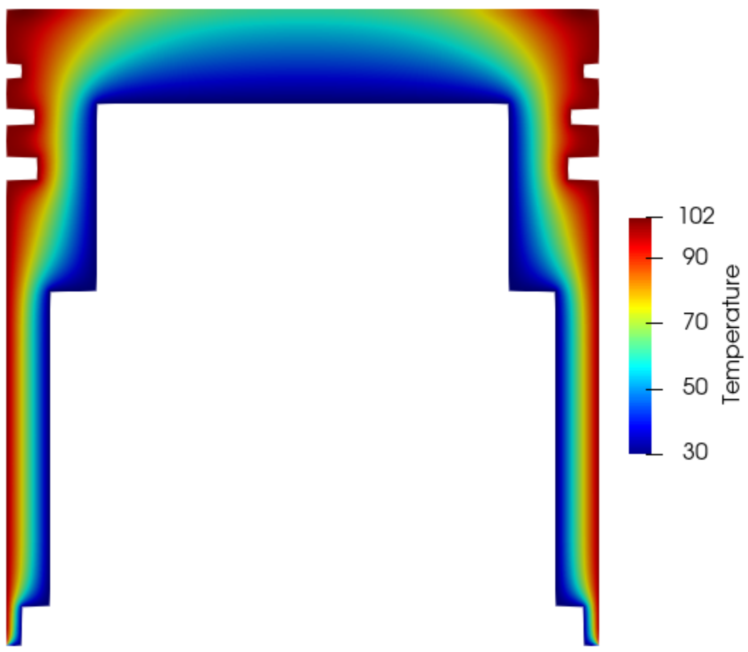
(c) Temperature distribution

Case 4.3 – 2D Piston

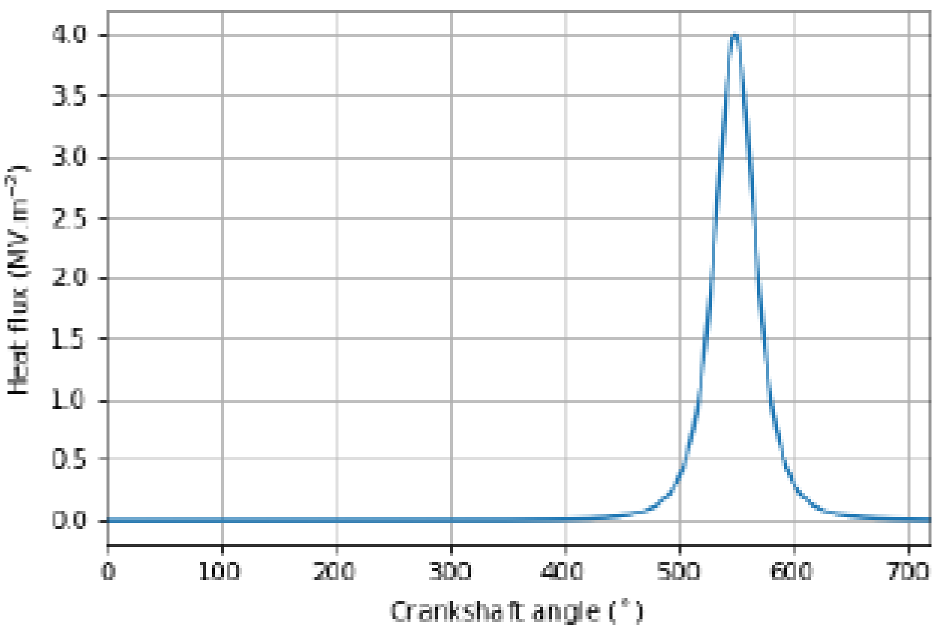
- Subcase 3: Time-dependent Neumann BC

Boundary ID	Comment	Type	Value	Unit
0	Top	Neumann	q_dot	$MW \cdot m^{-2}$
1	Liner	Dirichlet	100	°C
2	Piston underneath	Dirichlet	30	°C

T = 6 s
dt = 0.005 s

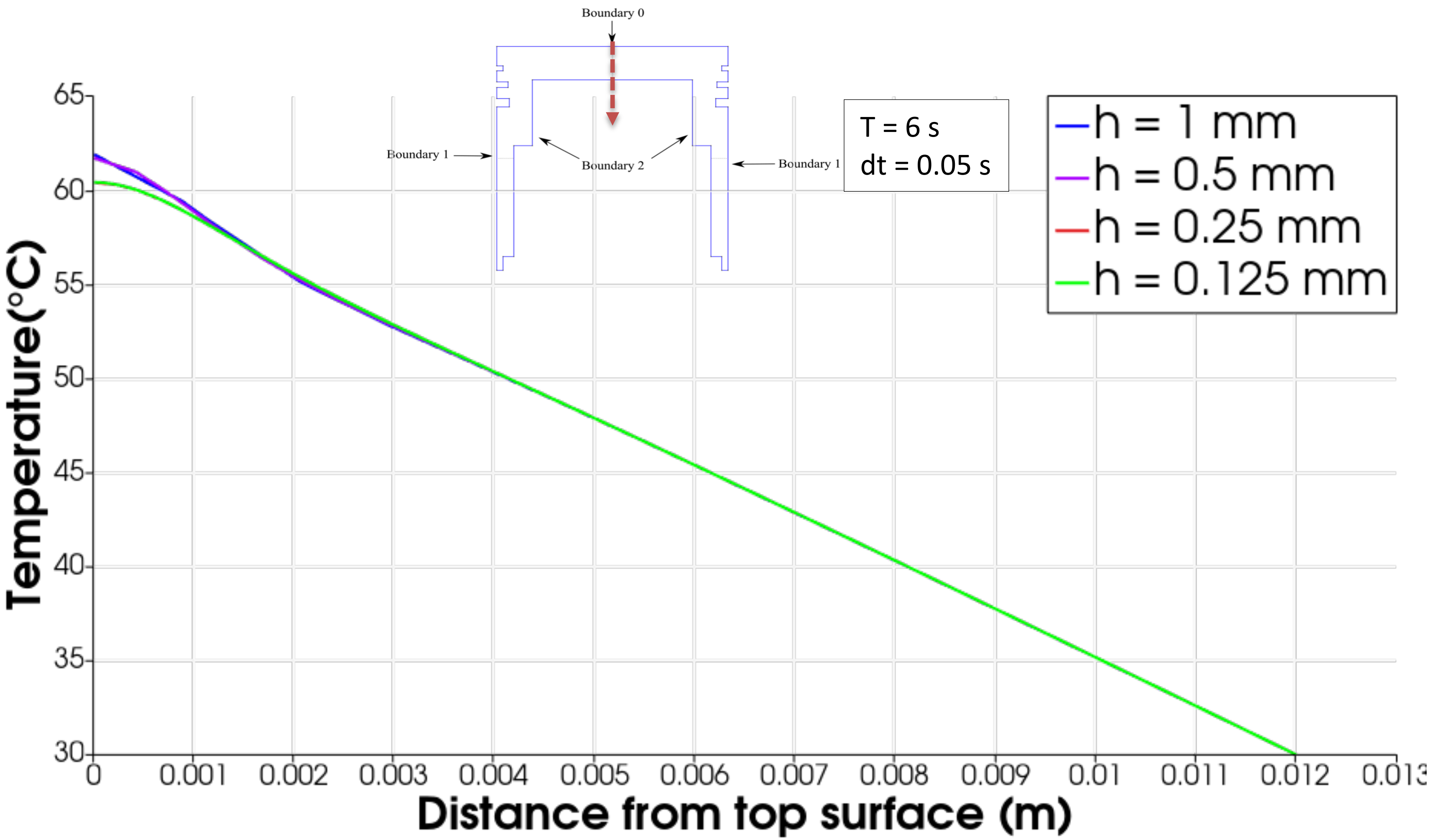


(a) Contour plot (h = 0.25mm)



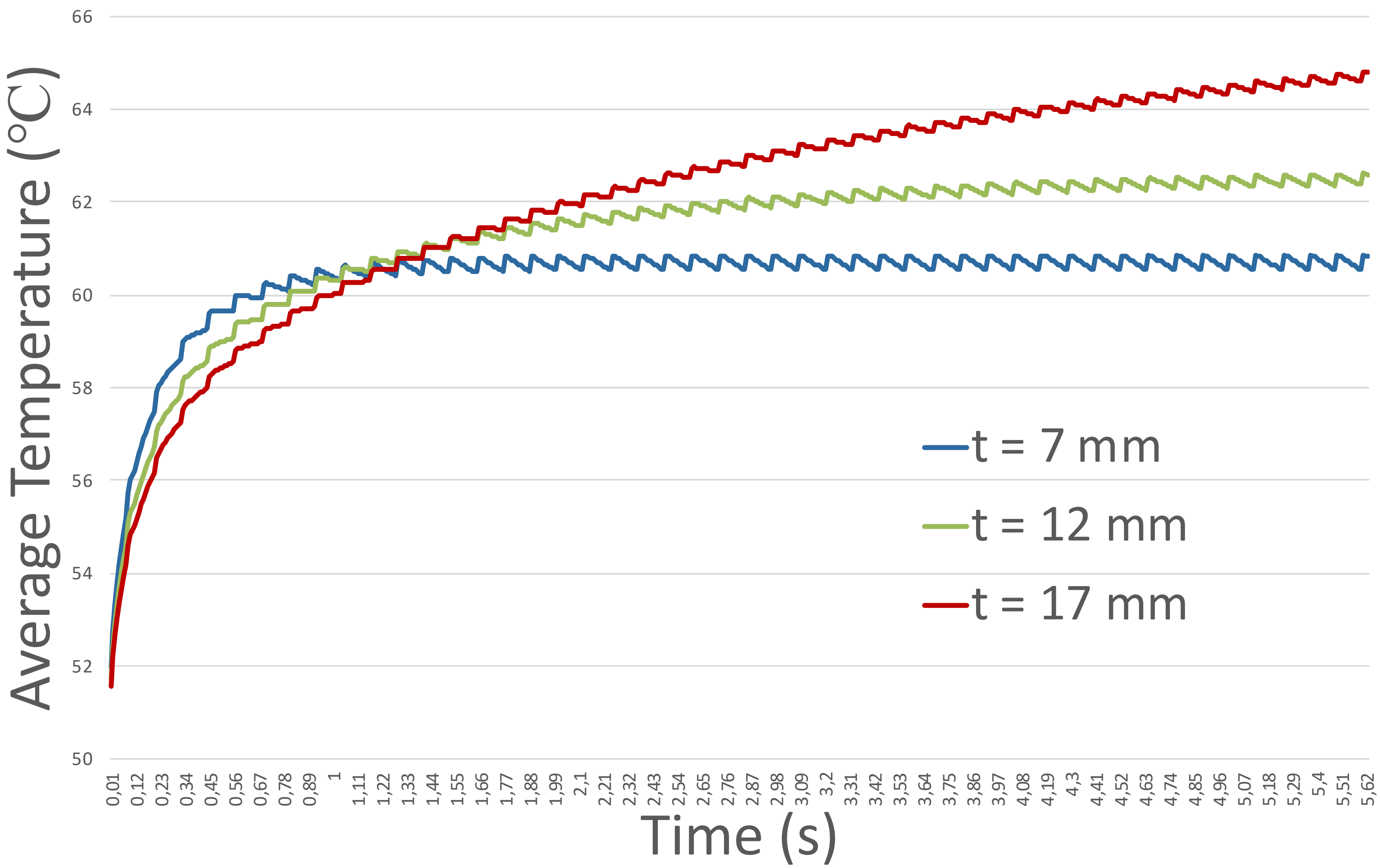
(b) Heat flux distribution for each piston cycle

Case 4.3 – 2D Piston – Mesh Convergence

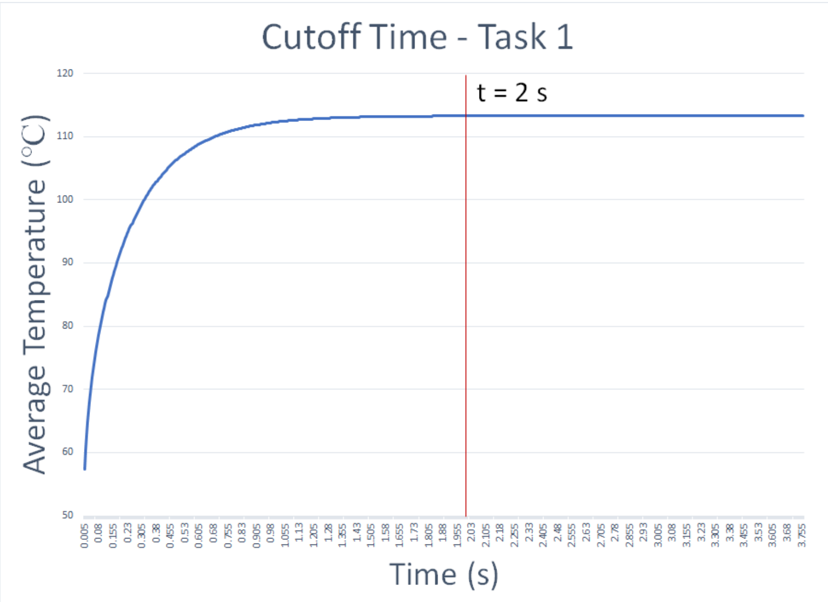


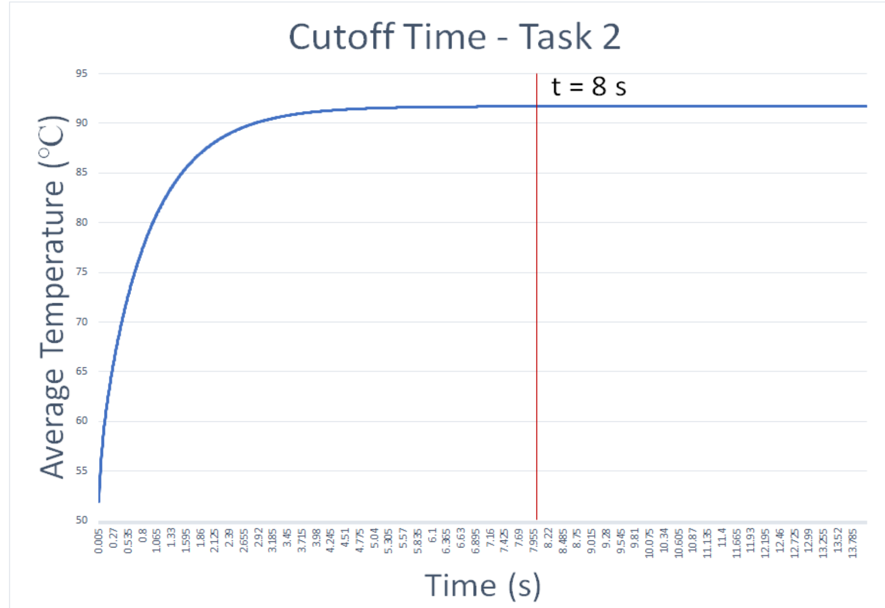
(c) Temperature distribution

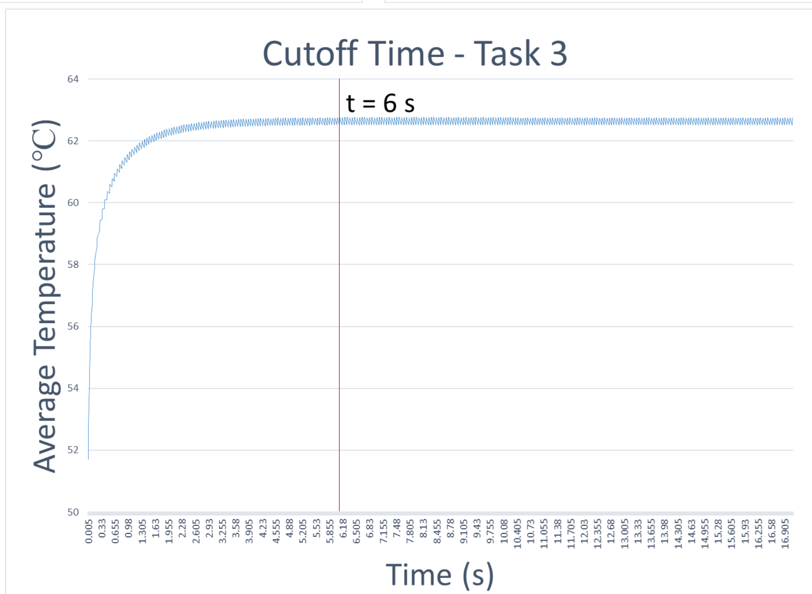
Case 4.3 – 2D Piston – Thickness study



Average Temperatures & Cutoff Times



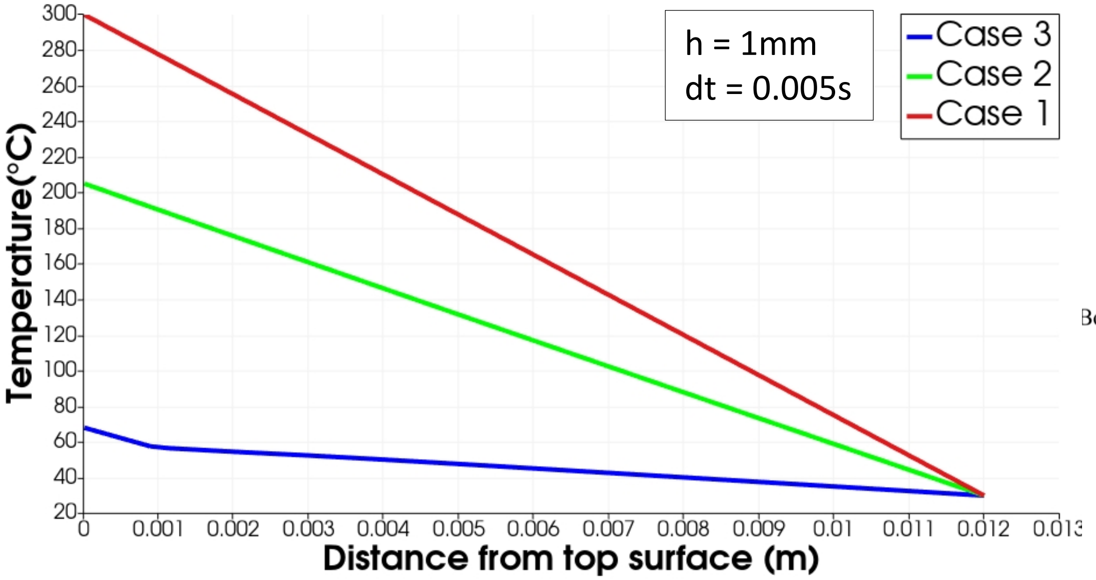




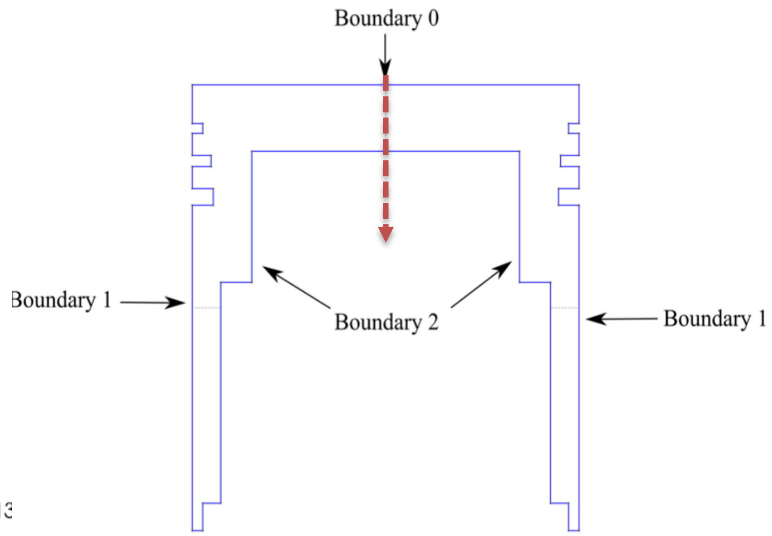
h = 1mm

Summary – 2D Piston

Temperature Distribution along the Vertical Line



(a) Temperature distribution



(b) Piston 2D setup

Summary – 2D Piston – Temperature

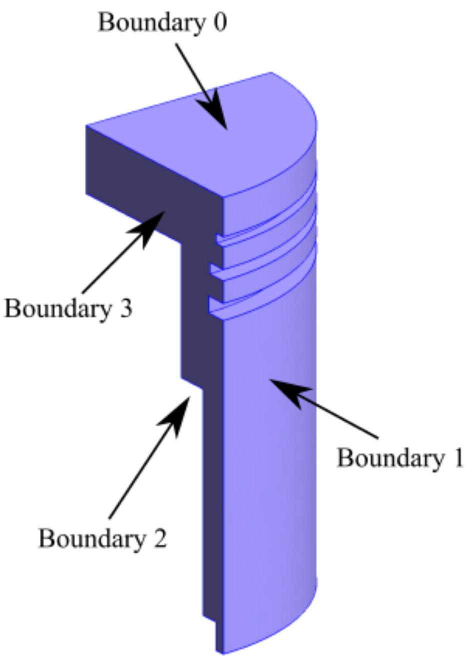
Task 1	MAX T (°C)	AVG T (°C)	MIN T (°C)
h = 10 mm	300.000	108.992	30.000
h = 5 mm	300.000	111.831	30.000
h = 1 mm	300.000	113.251	30.000

Task 2	MAX T (°C)	AVG T (°C)	MIN T (°C)
h = 10 mm	208.197	89.718	30.000
h = 5 mm	208.233	91.111	30.000
h = 1 mm	208.780	91.695	30.000

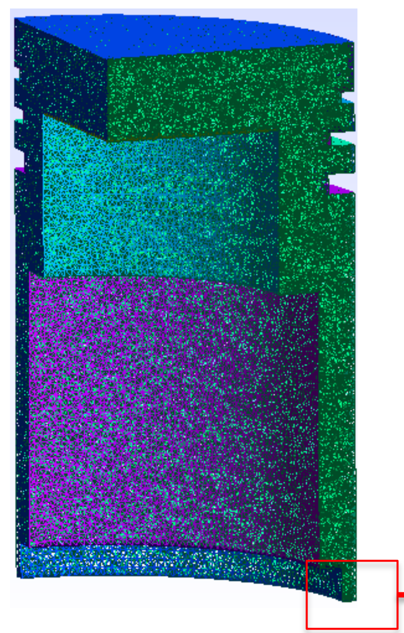
Task 3	MAX T (°C)	AVG T (°C)	MIN T (°C)
h = 1 mm	102.324	62.700	30.000
h = 0.5 mm	102.332	62.729	30.000
h = 0.25 mm	102.323	62.729	30.000

Case 4 – 3D Piston – Problem description

- **PDE:** Time-dependent Heat(Diffusion) Equation
- **Time Domain:** Unsteady (Transient)

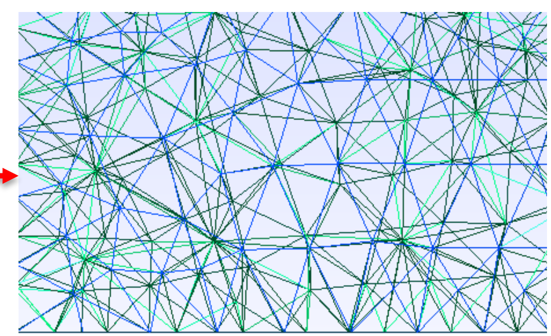


(a) 3D setup



(b) Meshed domain

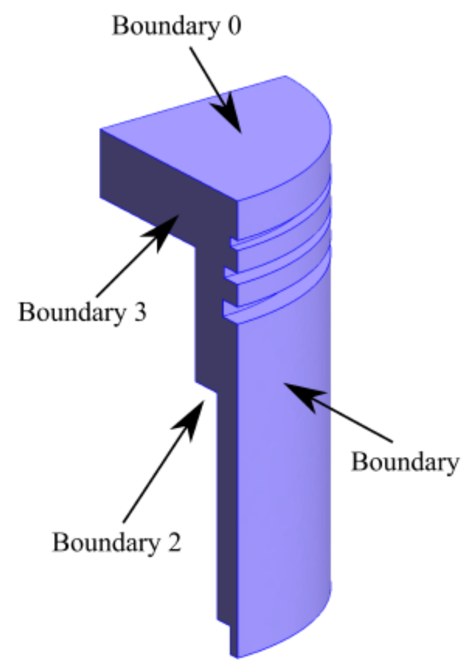
Mesh details:
Refinement level (h) = 1mm
No. of elements = 166681
No. of nodes = 35977



Case 4.1 – 3D Piston – Dirichlet BCs

- Boundary Conditions:

Boundary ID	Comment	Type	Value	Unit
0	Top	Dirichlet	300	°C
1	Liner	Dirichlet	100	°C
2	Piston underneath	Dirichlet	30	°C
3	Symmetry plane	Neumann	0	$W \cdot m^{-2}$



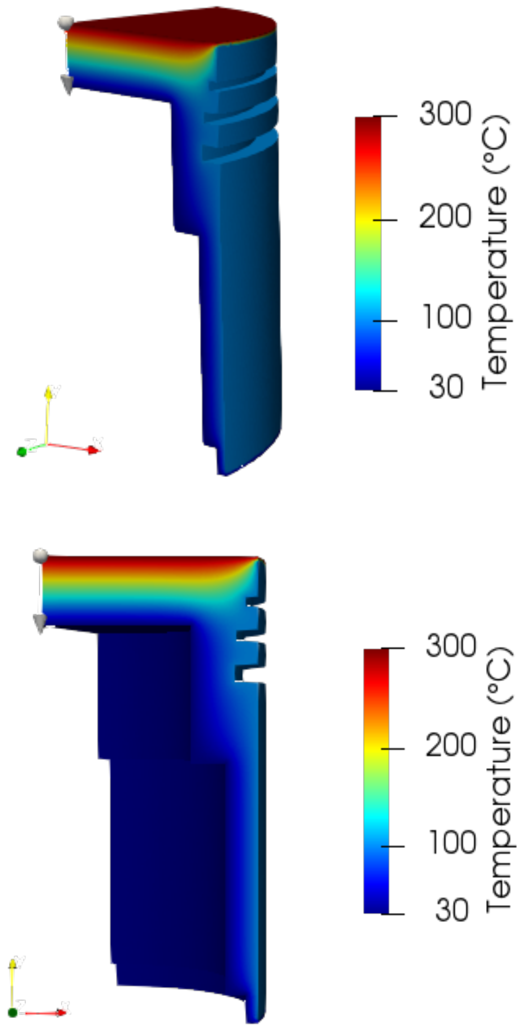
(c) Boundary conditions

- Weak form:

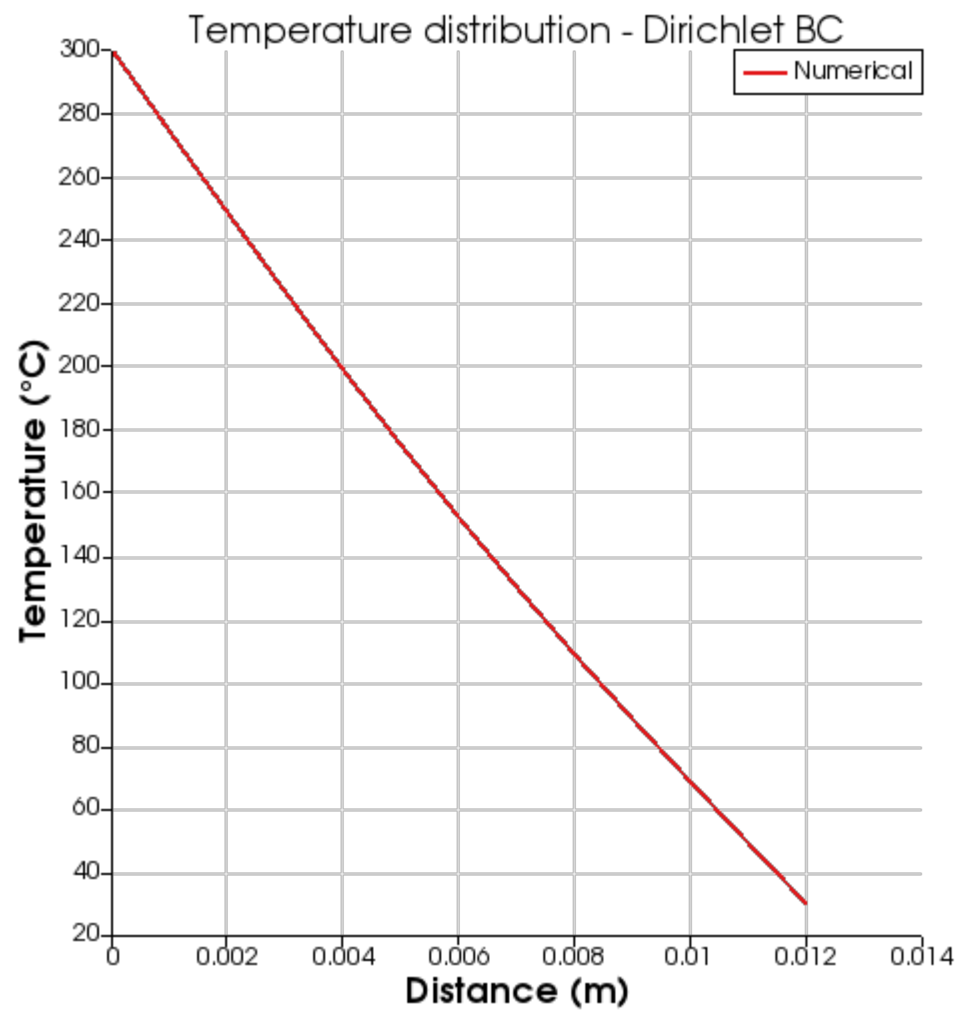
= 0

  – $\int_\Omega w\,T^{n+1} d\Omega - \int_\Omega w T^n d\Omega + \int_\Omega \Delta t\,(\alpha \nabla w . \nabla T^{n+1}) d\Omega - \cancel{\int_{\Gamma_n} \Delta t \frac{\alpha}{k} (\hat{n}.\vec{q})\ w\,d\Gamma} = 0$

Case 4.1 – 3D Piston – Results



(d) Contour plots

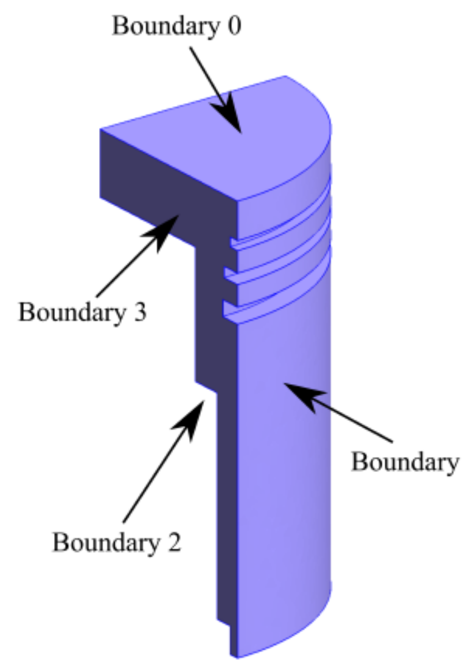


(e) Line plot

Case 4.2 – 3D Piston – Neumann BCs

- Boundary Conditions:

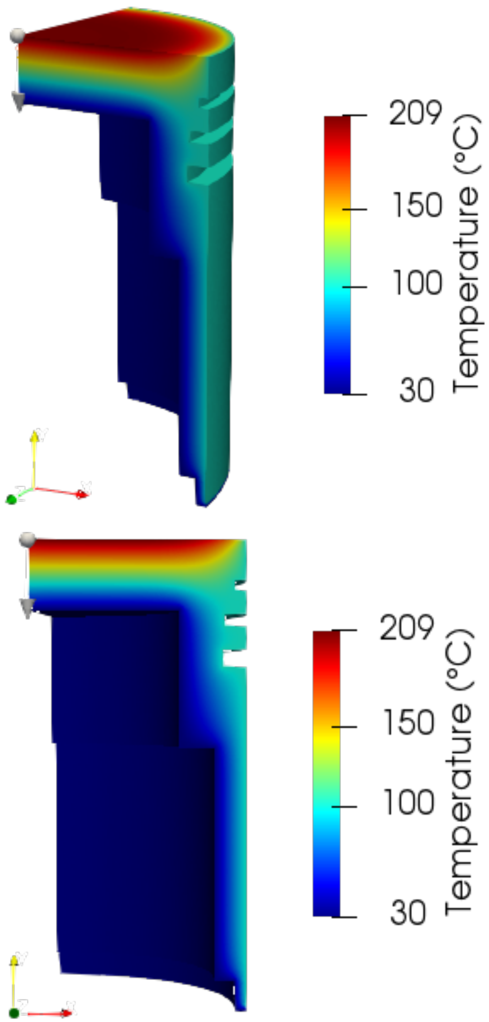
Boundary ID	Comment	Type	Value	Unit
0	Top	Neumann	2	$MW \cdot m^{-2}$
1	Liner	Dirichlet	100	°C
2	Piston underneath	Dirichlet	30	°C
3	Symmetry plane	Neumann	0	$W \cdot m^{-2}$



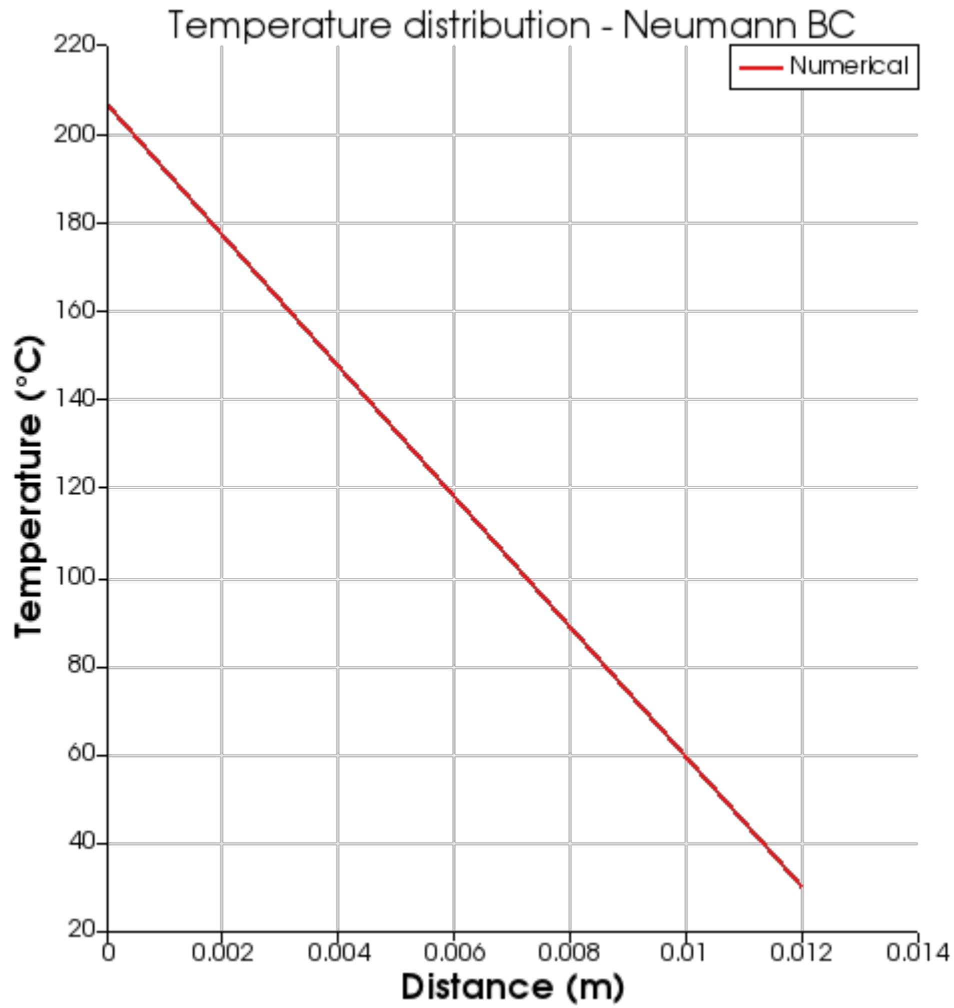
(a) Boundary conditions

- Weak form:
  – $\int_\Omega w\, T^{n+1} d\Omega - \int_\Omega w T^n d\Omega + \int_\Omega \Delta t\,(\alpha \nabla w . \nabla T^{n+1}) d\Omega - \boxed{\int_{\Gamma_n} \Delta t \frac{\alpha}{k} (\hat{n}.\vec{q})\; w\, d\Gamma} = 0$

Case 4.2 – 3D Piston – Results



(b) Contour plots

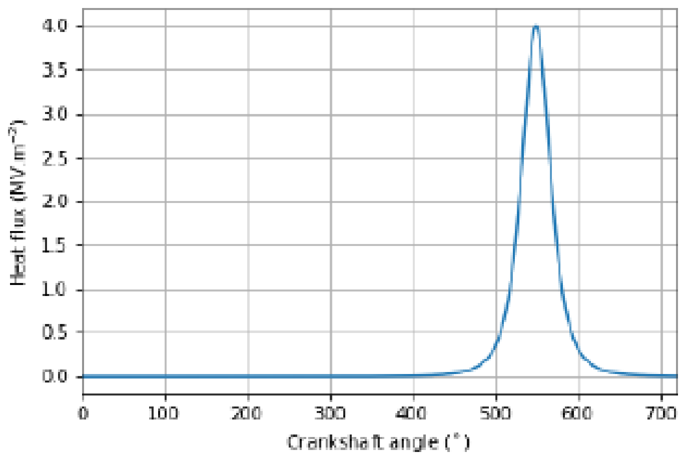


(c) Line plot

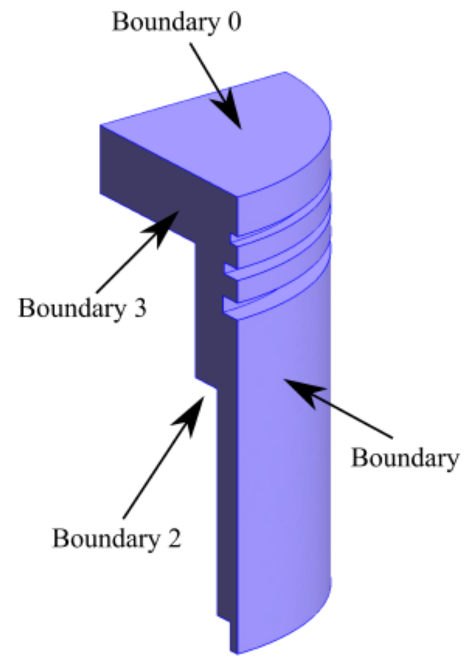
Case 4.3 – 3D Piston – Time dependent BC

- Boundary Conditions:

Boundary ID	Comment	Type	Value	Unit
0	Top	Neumann	q_dot	$MW \cdot m^{-2}$
1	Liner	Dirichlet	100	°C
2	Piston underneath	Dirichlet	30	°C
3	Symmetry plane	Neumann	0	$W \cdot m^{-2}$



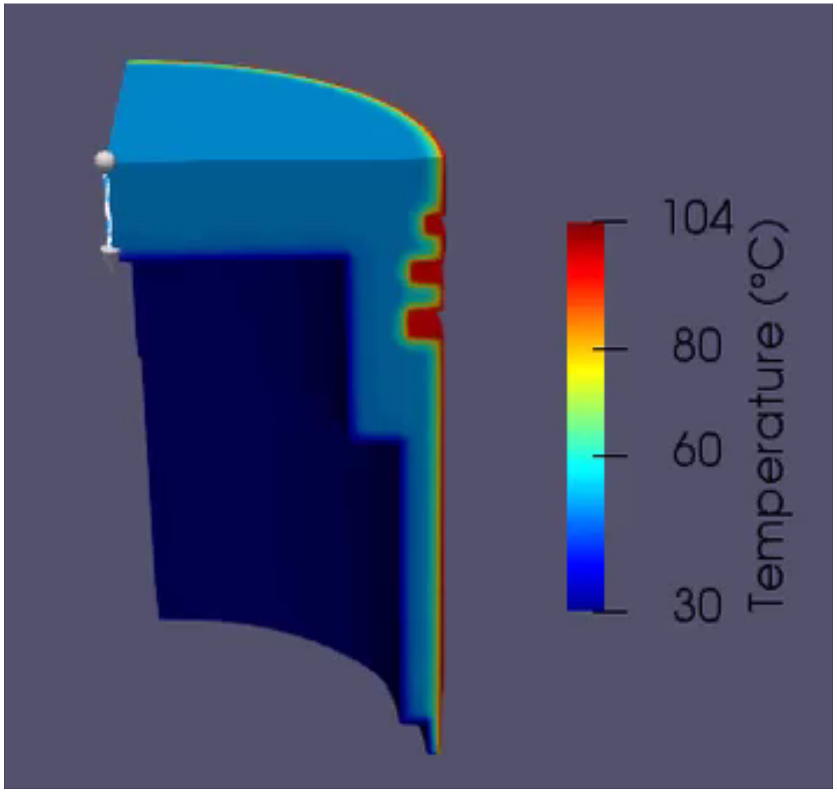
(b) Time dependent Heat flux



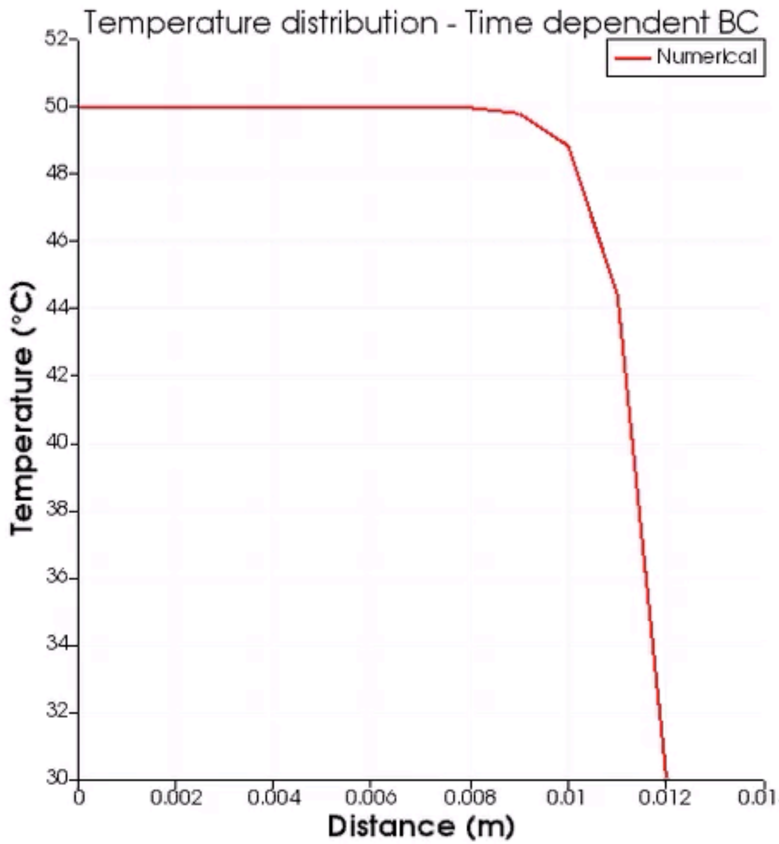
(a) Boundary conditions

- Weak form:
  - $$\int_{\Omega} w\, T^{n+1} d\Omega - \int_{\Omega} w T^{n} d\Omega + \int_{\Omega} \Delta t\, (\alpha \nabla w . \nabla T^{n+1}) d\Omega - \boxed{\int_{\Gamma_n} \Delta t \frac{\alpha}{k} (\hat{n} . \vec{q})\ w\, d\Gamma} = 0$$

Case 4.3 – 3D Piston – Results

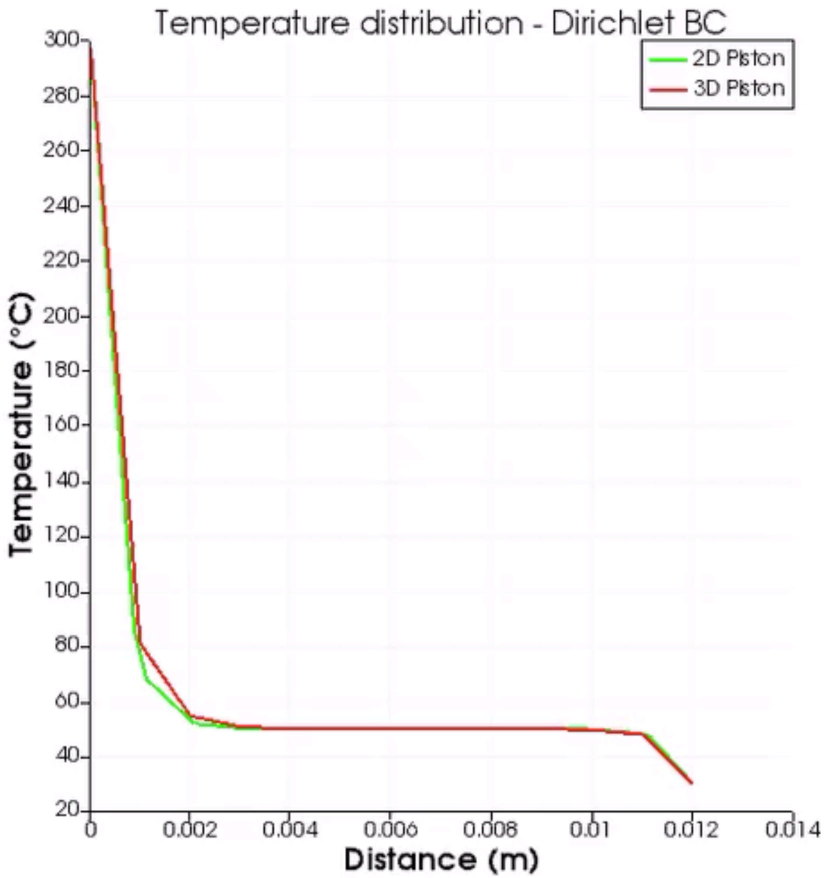


(c) Contour plot

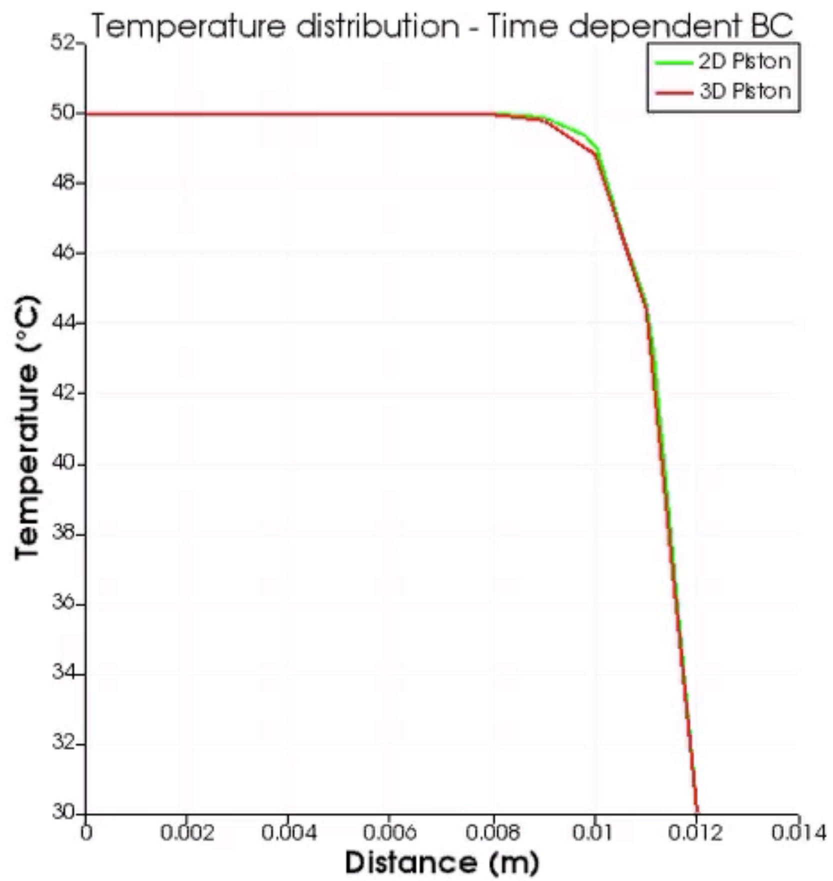


(d) Line plot

Case 4 – 3D vs. 2D Comparison



(a) Dirichlet BC

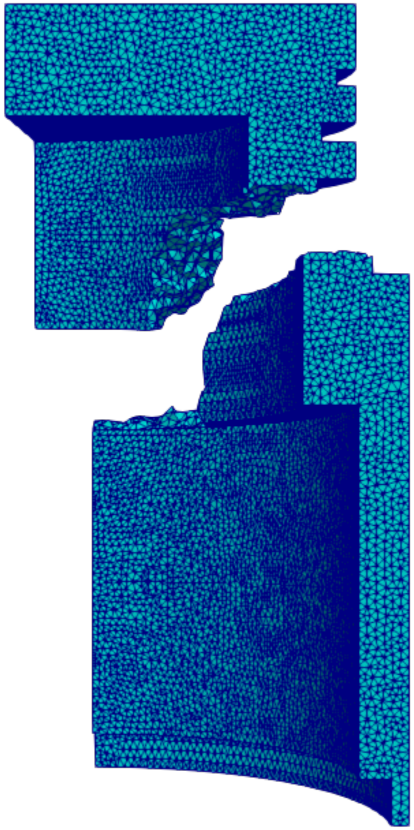


(b) Time dependent Heat flux

Case 4 – 3D Piston – MPI

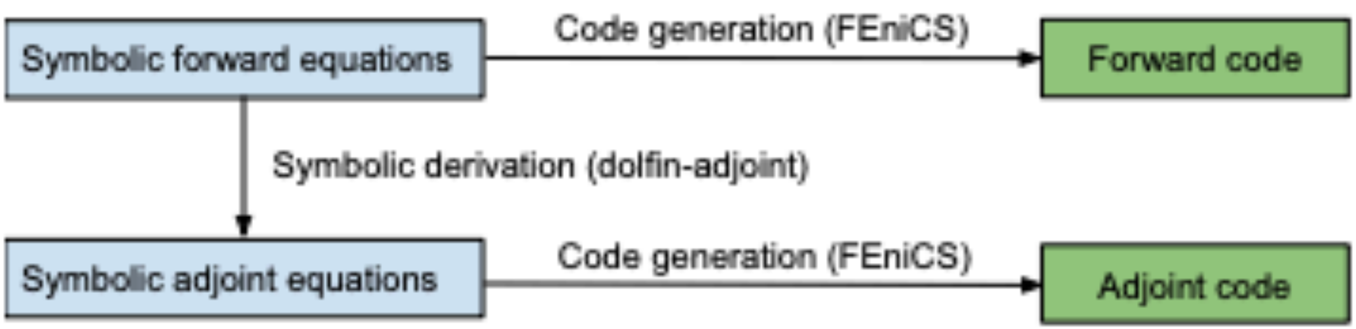
No. of processors	Time (Sec)	Speedup	Parallel Efficiency
Sequential	248	-	-
2	133	1.86	0.93
3	120	2.06	0.68
4	111	2.23	0.55

(a) MPI Timings



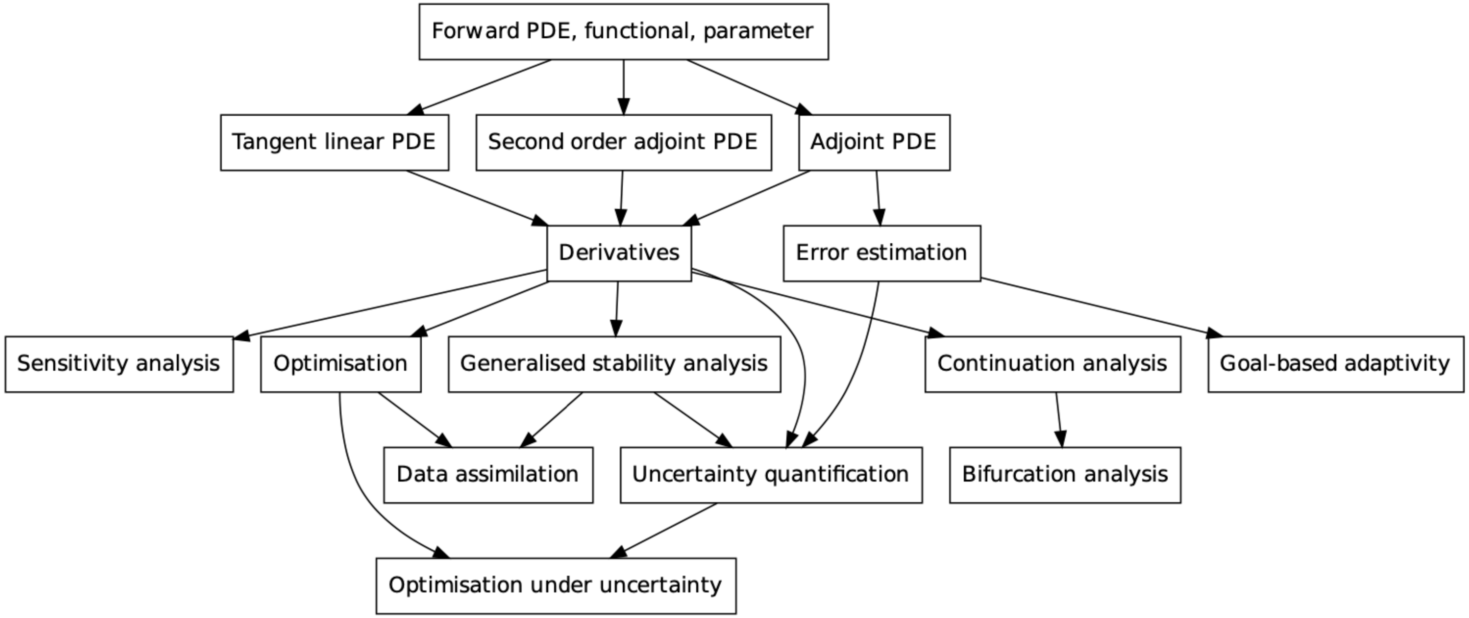
(b) Domain partition (np = 2)

FEniCS Dolfin-Adjoint



Computing sensitivity

- Sensitivity with respect to certain parameters
  - Initial conditions,
  - Forcing terms,
  - Unknown coefficients.

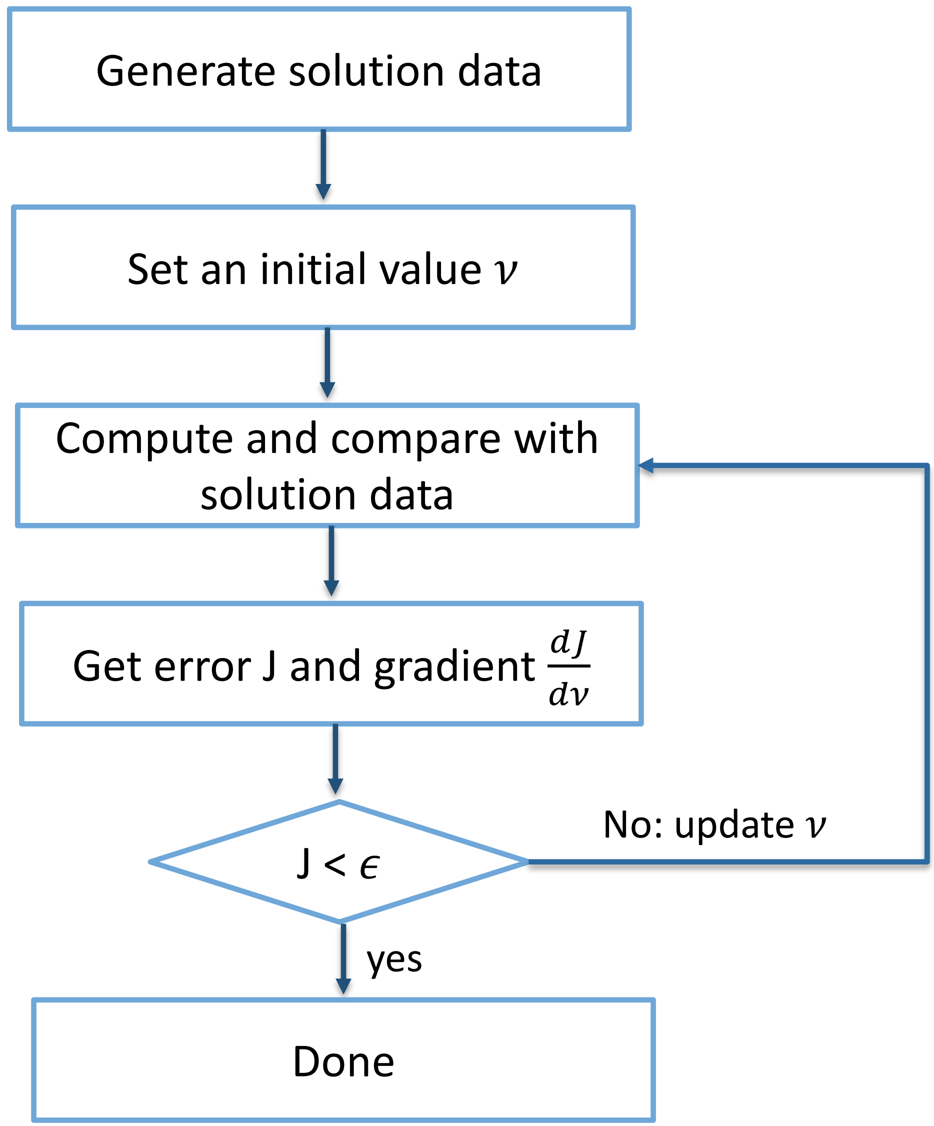


Case 5 – Algorithmic differentiation

- **Steps**
  - $J(u) = \int_\Omega < u_{red}(T) - u(T), u_{red}(T) - u(T) > d\Omega$
  - Calculate Jacobian $\frac{dJ}{d\nu}$
  - Update: $\nu = \nu - \alpha \frac{dJ}{d\nu}$

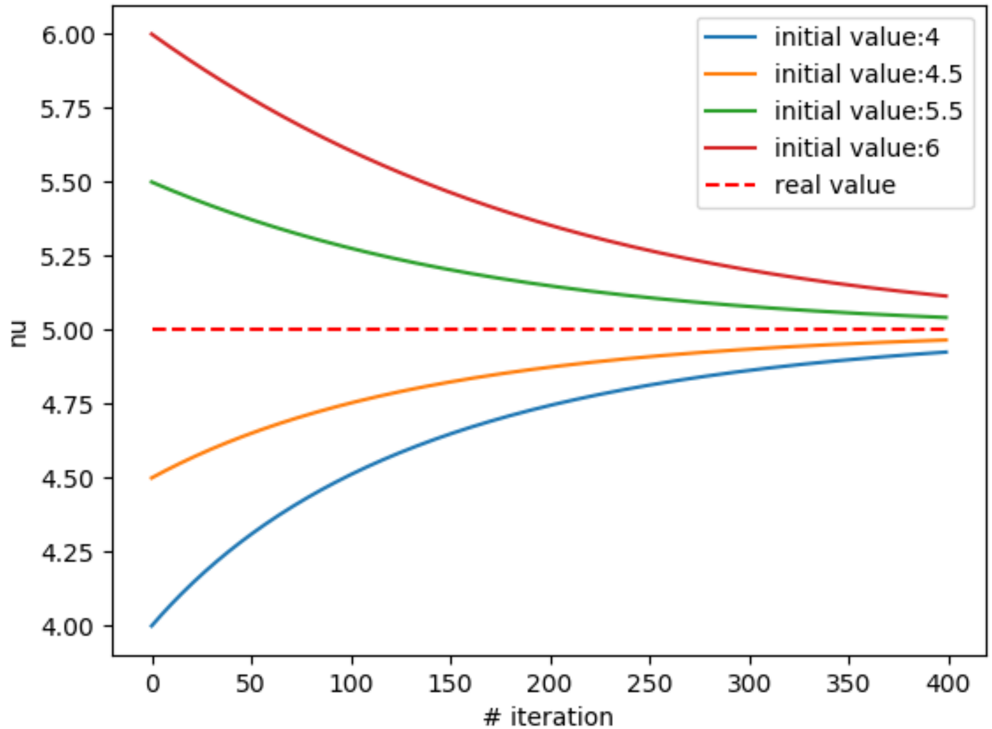
- **Tasks**
  - Confirm the code works
  - Sensitivity analysis
    - α (step-size)
    - Mesh size

Case 5 - Algorithmic differentiation



Case 5 - Algorithmic differentiation

- Confirm (2D Square)
  - Step size (α) : 0.5; Exact value : 5.00

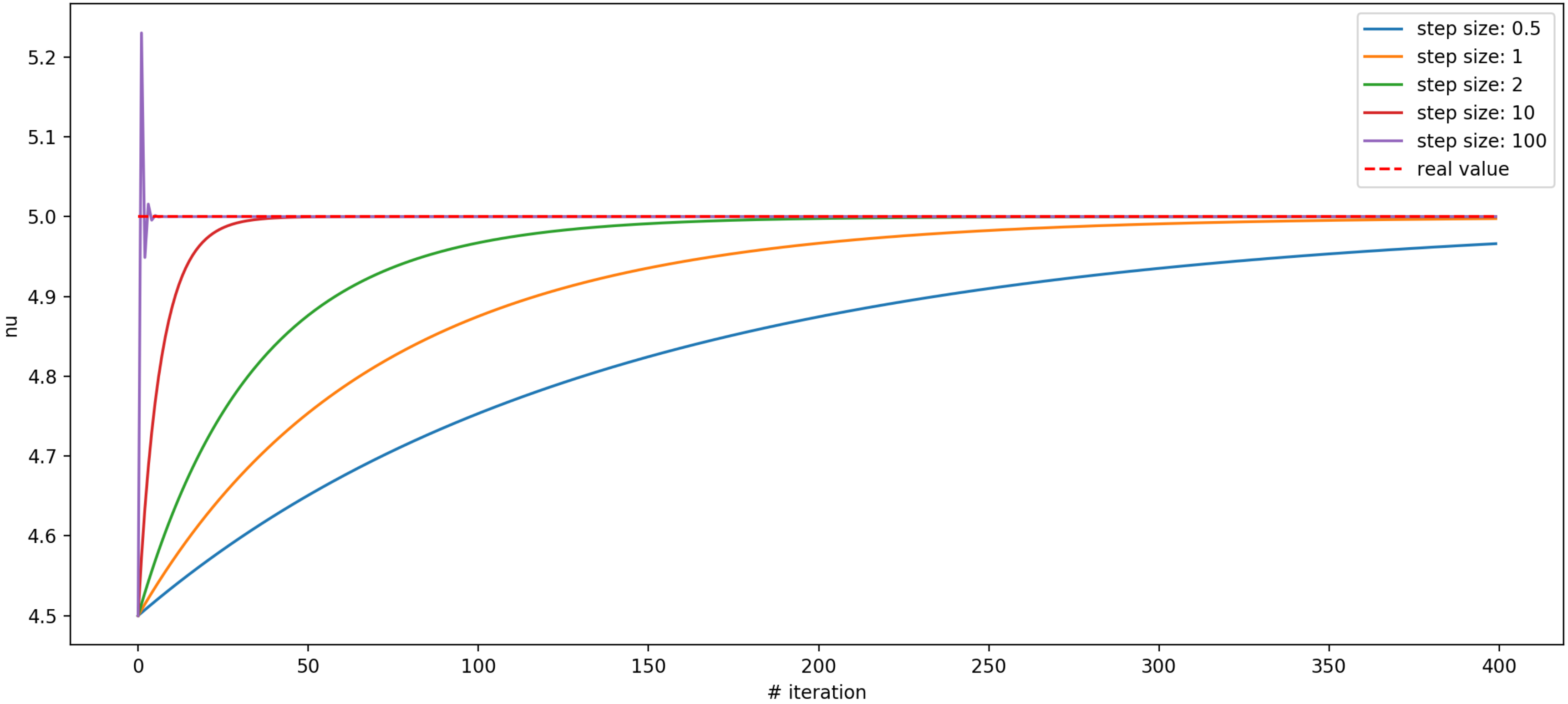


Test convergence of different initial values

Results	
Initial Value	**Estimation Value**
4.00	4.925
4.50	4.966
5.50	5.042
6.00	5.115

Case 5 - Algorithmic differentiation

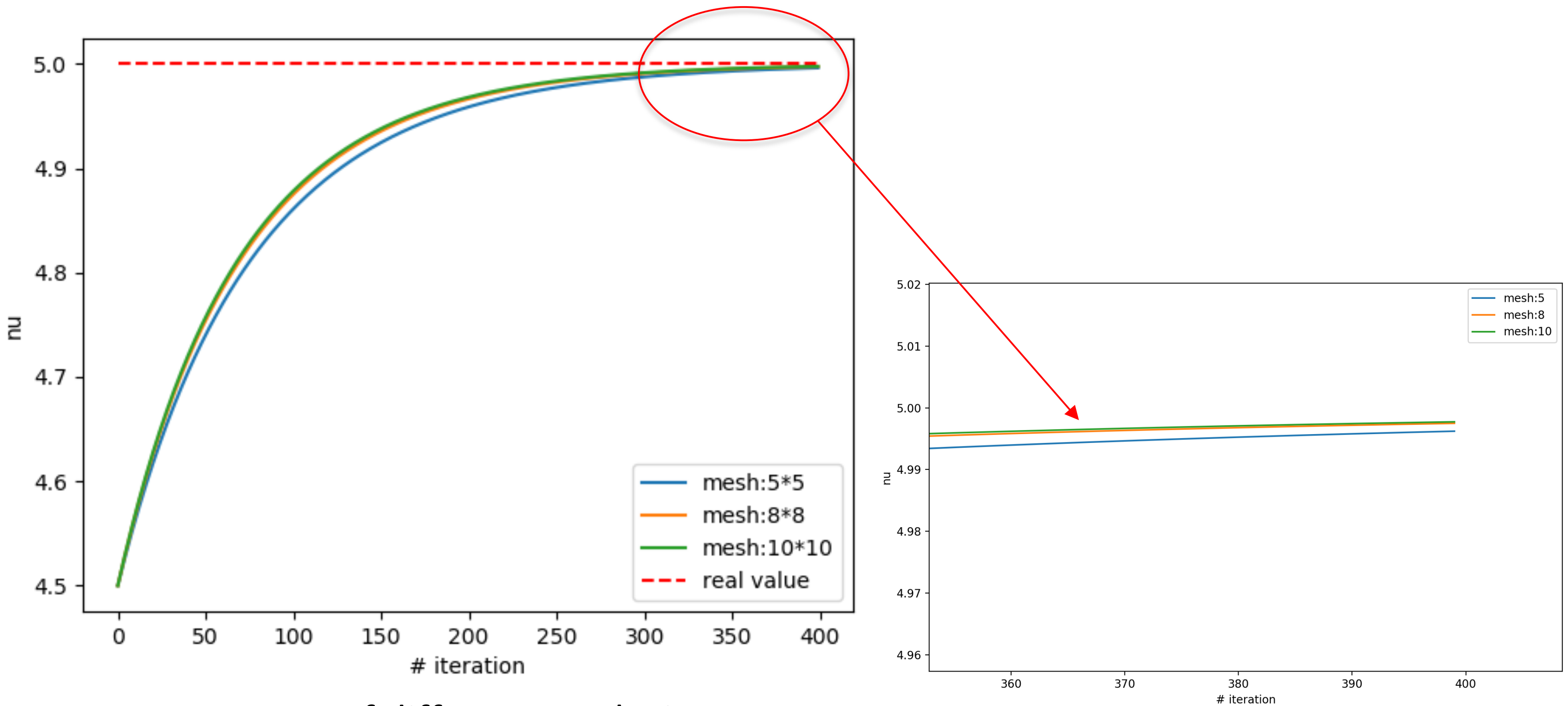
- Step size effect (2D Square)
  - Initial value : 4.50; Exact value : 5.00



Step size (α) effect for convergence

Case 5 - Algorithmic differentiation

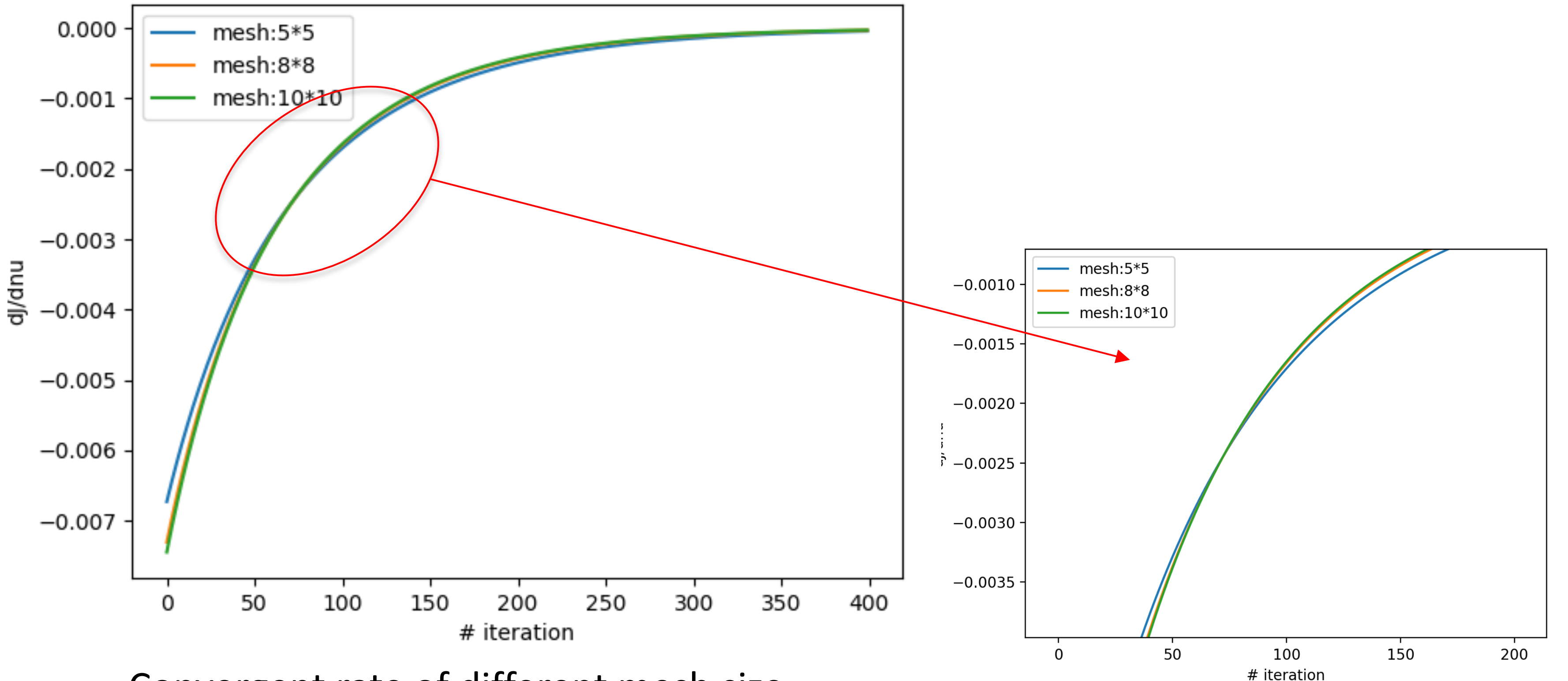
- Mesh size effect (2D Square)
  - Step size (α) : 1; Initial value : 4.50; Exact value : 5.00



ν convergence of different mesh size

Case 5 - Algorithmic differentiation

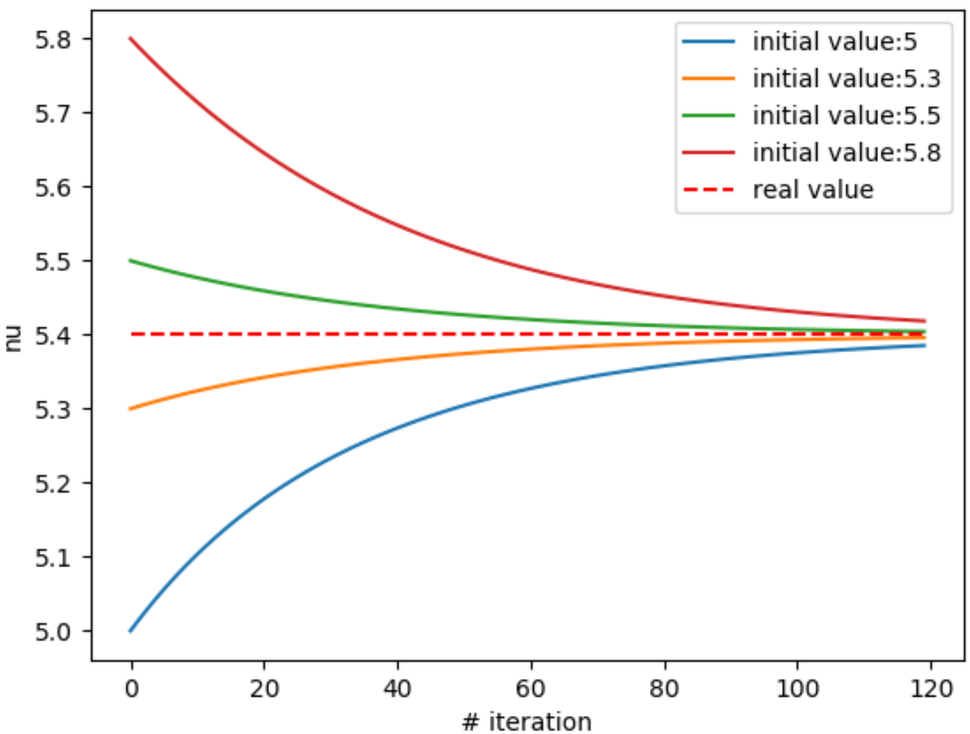
- Mesh size effect (2D Square)
  - Step size (α) : 1; Initial value : 4.50; Exact value : 5.00



Convergent rate of different mesh size

Case 5 - Algorithmic differentiation

- Confirm (2D Piston)
  - Step size (α) : 1;   Exact value : 5.40

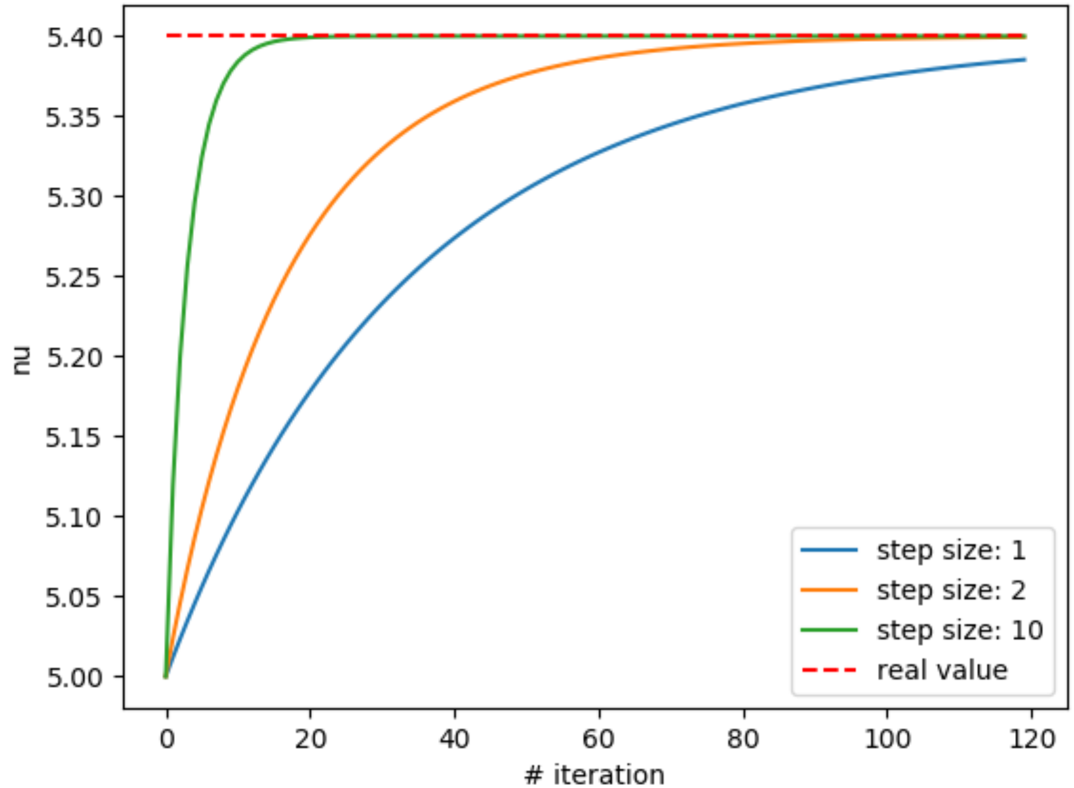


Test convergence of different initial value

Results	
Initial Value	**Estimation Value**
5.00	5.385
5.30	5.396
5.50	5.404
5.80	5.419

Case 5 - Algorithmic differentiation

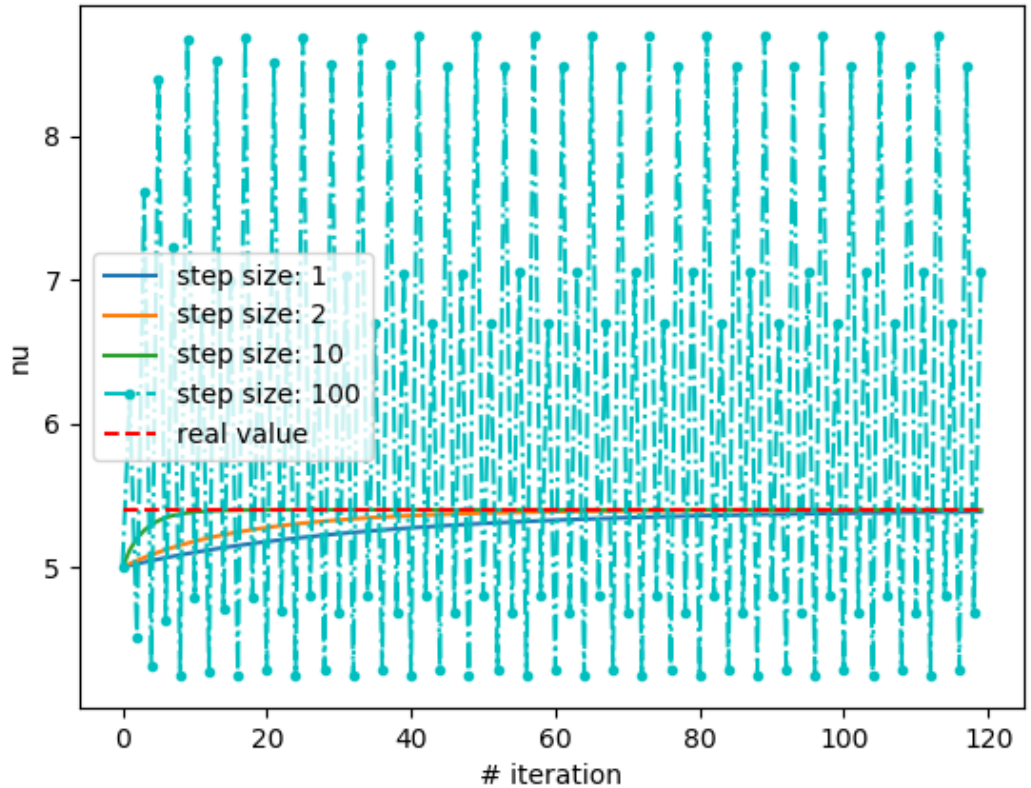
- Step size effect (2D Piston)
  - Initial value : 5.00; Exact value : 5.40



Step size (α) effect for convergence

Case 5 - Algorithmic differentiation

- Step size effect (2D Piston)
  - Initial value : 5.00; Exact value : 5.40



Step size (α) effect for convergence

Conclusion

- FEM, and FEniCS to solve 5 different cases
- We now have validated diffusion solvers that could readily be used for any heat transfer application.
- Further exploration points:
  - Case 4.3 Piston: optimize step size
  - Parallelization in cluster
  - Case 5 AD: investigate impact of step size α

Reference

- https://fenicsproject.org/
- Anders Logg, Kent-Andre Mardal, Garth N. Wells: Automated Solution of Differential Equations by the Finite Element Method. fenicsproject.org, 2011.
- Roland W. Lewis, Perumal Nithiarasu, Kankanhalli N. Seetharamu:Fundamentals of the Finite Element Method for Heat and Fluid Flow. John Wiley Sons, 2004.
- Axel Gerstenberger. An XFEM based fixed-grid approach to fluid-structure interac- tion. PhD thesis, Ph. D. Thesis, 2010.

Project Management

Team Member	Main Responsibility
AHN, Na Young	Project Management, Overview, Visualisation
NAGESH, Manoj Cendrollu	Main Developer, Case 4 3D Piston, Case 5 AD, MPI
VELIOGLU, Mehmet	Main Developer, Case 4 2D Piston
WU, Zhao	Main Developer, Case 5 AD

Any Burning Questions?