Enriched Finite Elements for Wave Propagation and Heat Diffusion using the Partition of Unity Method

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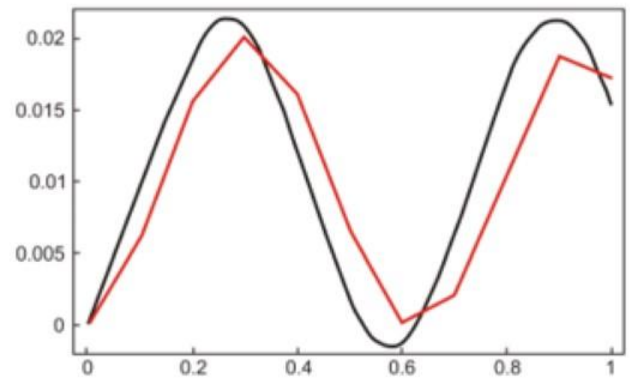
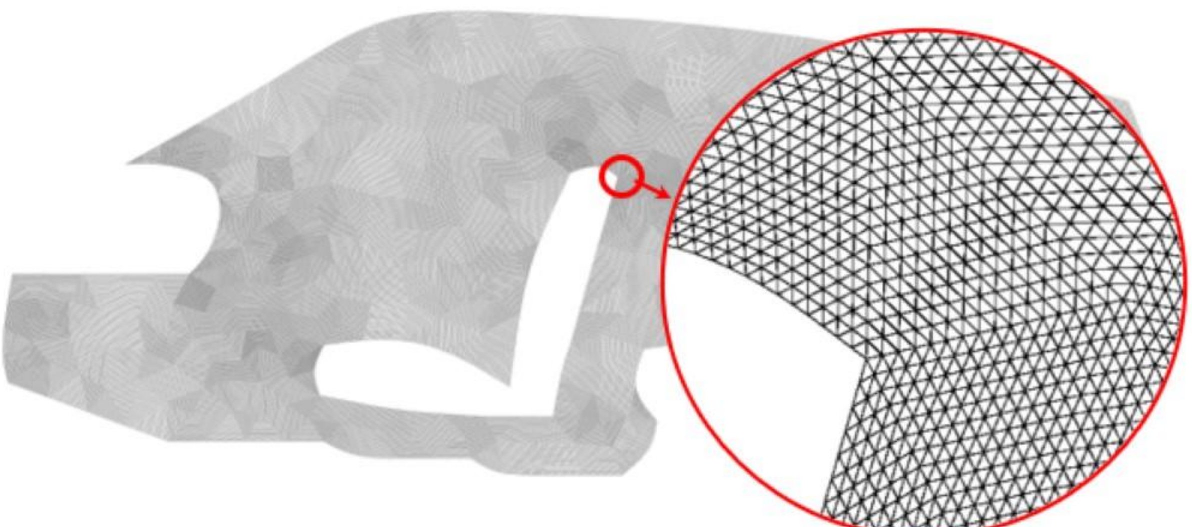
Wave problem

1.0 Wave problem



polynomials requires many nodes wavelength.

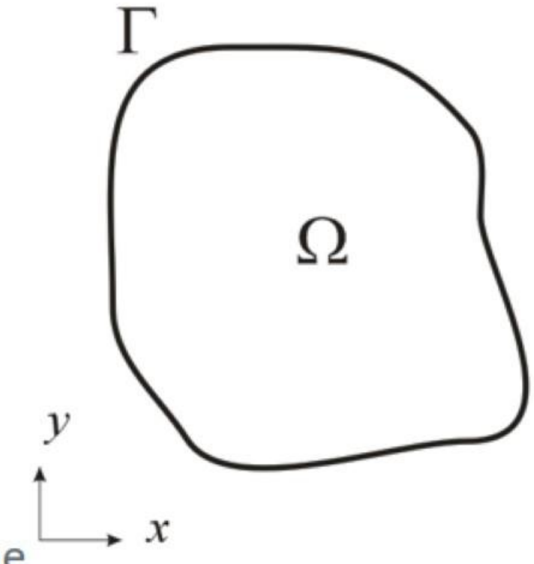
If you increase the wavenumber increases more nodes are needed (pollution error).



1.1 Wave problem

We define the following initial value problem with the wave equation and a set of initial and boundary conditions:

$$
\begin{aligned}
\frac{\partial^2 E}{\partial t^2} - c^2 \nabla^2 E &= f(t, \mathbf{x}), \qquad (t, \mathbf{x}) \in [0, T[\times \Omega, \\
\frac{\partial E}{\partial \hat{\mathbf{v}}} + hE &= g(t, \mathbf{x}), \qquad (t, \mathbf{x}) \in [0, T[\times \Gamma, \\
E(0, \mathbf{x}) &= E^0(\mathbf{x}), \qquad \mathbf{x} \in \Omega, \\
\frac{\partial E}{\partial t}(0, \mathbf{x}) &= V^0(\mathbf{x}), \qquad \mathbf{x} \in \Omega,
\end{aligned}
$$



The problem is defined over the domain Ω and the time interval $[0, T[$. We first discretise the problem in time using the second-order central difference method:

$$
\begin{aligned}
\frac{E^{n+1} - 2E^n + E^{n-1}}{\Delta t^2} - c^2 \nabla^2 E^{n+1} &= f(t_{n+1}, \mathbf{x}), \qquad n = 0, 1, 2, \ldots, \\
E^0(\mathbf{x}) &= E^0(\mathbf{x}), \\
E^{-1}(\mathbf{x}) &= E^0(\mathbf{x}) - \Delta t V^0(\mathbf{x}).
\end{aligned}
$$

2.0 Weak formulation

Applying the **divergence theorem** and substituting the **boundary conditions** we get the following standard weak formulation:

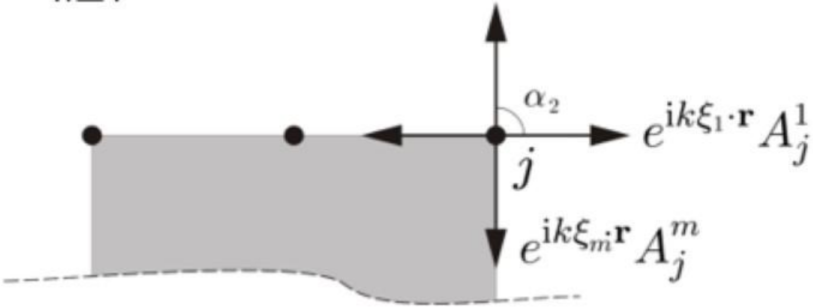
$$\int_\Omega E^{n+1}\phi \, d\Omega + (c^2\Delta t^2)\int_\Omega \nabla E^{n+1}\cdot\nabla\phi \, d\Omega + (c^2\Delta t^2)\oint_\Gamma (hE^{n+1})\phi \, d\Gamma =$$
$$\int_\Omega \Big(2E^n - E^{n-1} + (\Delta t^2) f(t_{n+1},\mathbf{x})\Big)\phi \, d\Omega + (c^2\Delta t^2)\oint_\Gamma g(t_{n+1},\mathbf{x})\phi \, d\Gamma$$

To solve the problem using **the finite element method**:

$$E_h^{n+1}(\mathbf{x}) = \sum_{j=1}^{N_d} E_j^{n+1}\mathcal{N}_j(\mathbf{x})$$

To solve the problem using the partition of unity finite element method

$$E_h^{n+1}(\mathbf{x}) = \sum_{i=1}^{M}\mathcal{N}_i\left(B_i^{n+1} + \sum_{q=1}^{Q-1} A_i^{q,n+1}\, e^{\mathrm{i}k\,(x\cos\alpha_q + y\sin\alpha_q)}\right)$$



3.0 Enriched approximation

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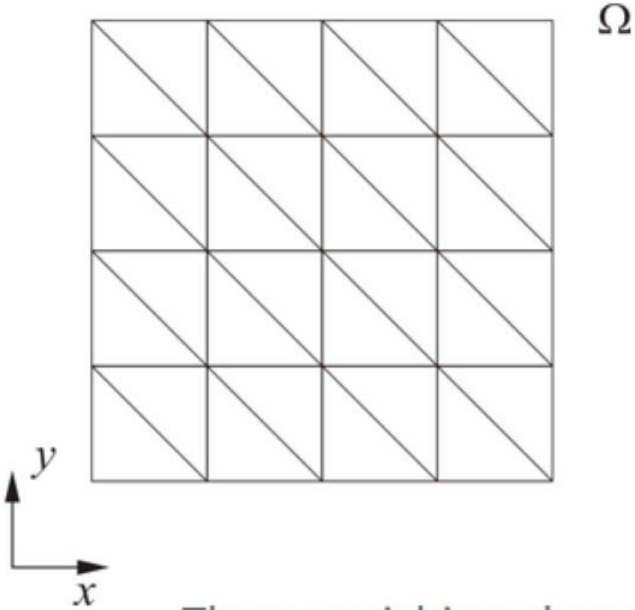
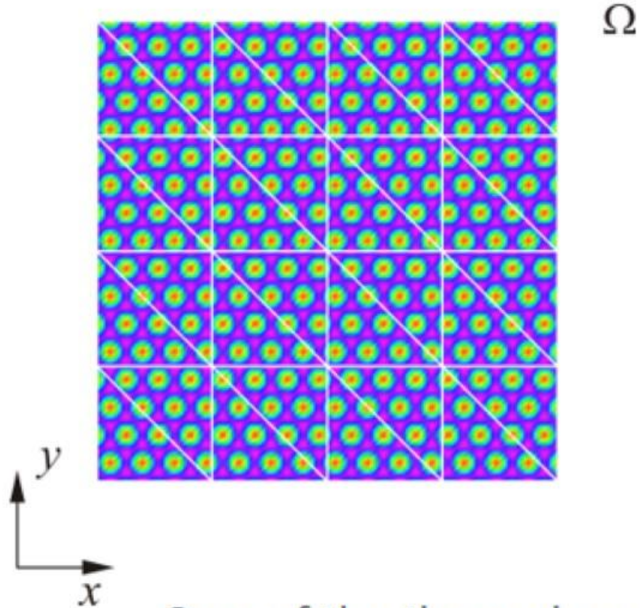
computational domain FE mesh

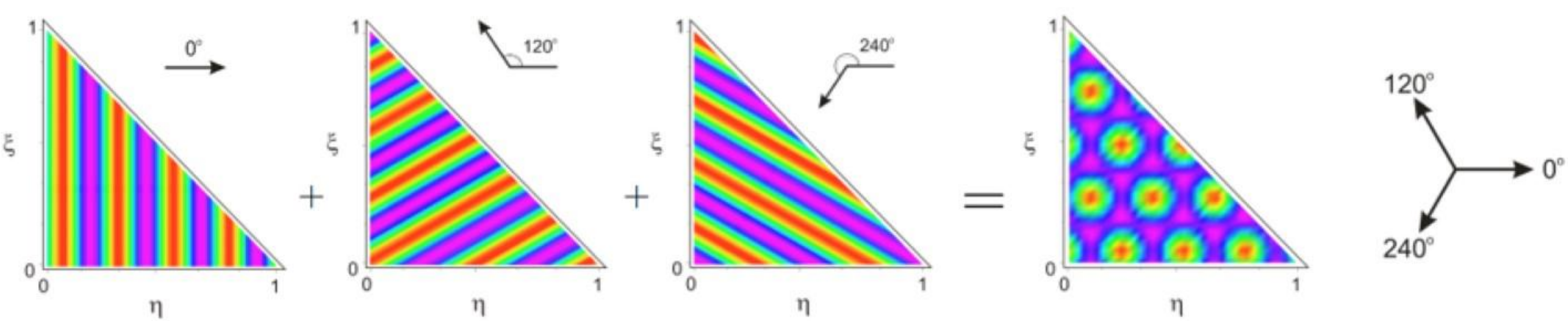


Computational domain enriched mesh



Three enriching plane waves

Sum of the three plane waves



4.0 Linear system

The assembled linear system is M x M blocks

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & \ldots & \mathcal{A}_{1M} \\ \mathcal{A}_{21} & \mathcal{A}_{22} & \ldots & \mathcal{A}_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{A}_{M1} & \mathcal{A}_{M2} & \ldots & \mathcal{A}_{MM} \end{pmatrix} \begin{Bmatrix} \mathbf{E}_1 \\ \mathbf{E}_2 \\ \vdots \\ \mathbf{E}_M \end{Bmatrix} = \begin{Bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \mathbf{b}_M \end{Bmatrix}$$

Each of the blocks ($\mathcal{A}_{11}$) corresponds to one of the mesh nodes $(1,1)$.

4.1 Linear system

The size of these blocks is Q x Q entries. Each block is associated with Q unknowns and Q entries of the load vector. One of the unknowns/load vector entries correspond to the constant enrichment function.

$$\mathcal{A}_{ij} = \begin{pmatrix} a_{ij}^{11} & a_{ij}^{12} & \dots & a_{ij}^{1Q} \\ a_{ij}^{21} & a_{ij}^{22} & \dots & a_{ij}^{2Q} \\ \vdots & \vdots & \ddots & \vdots \\ a_{ij}^{Q1} & a_{ij}^{Q2} & \dots & a_{ij}^{QQ} \end{pmatrix} \quad \mathbf{E}_j = \begin{Bmatrix} B_j^{n+1} \\ A_j^{2,n+1} \\ \vdots \\ A_j^{Q,n+1} \end{Bmatrix} \quad \mathbf{b}_j = \begin{Bmatrix} b_j^1 \\ b_j^2 \\ \vdots \\ b_j^Q \end{Bmatrix}$$

5.0 Example 1

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In the first test example we consider a circular wave in a unity square domain. The wave is defined by

$$\widetilde{E}(t,x,y) = e^{\mathrm{i}(kr-\omega t)}$$

where we take $\omega = 1$. Based on the above exact form we can then obtain the initial velocity and displacements

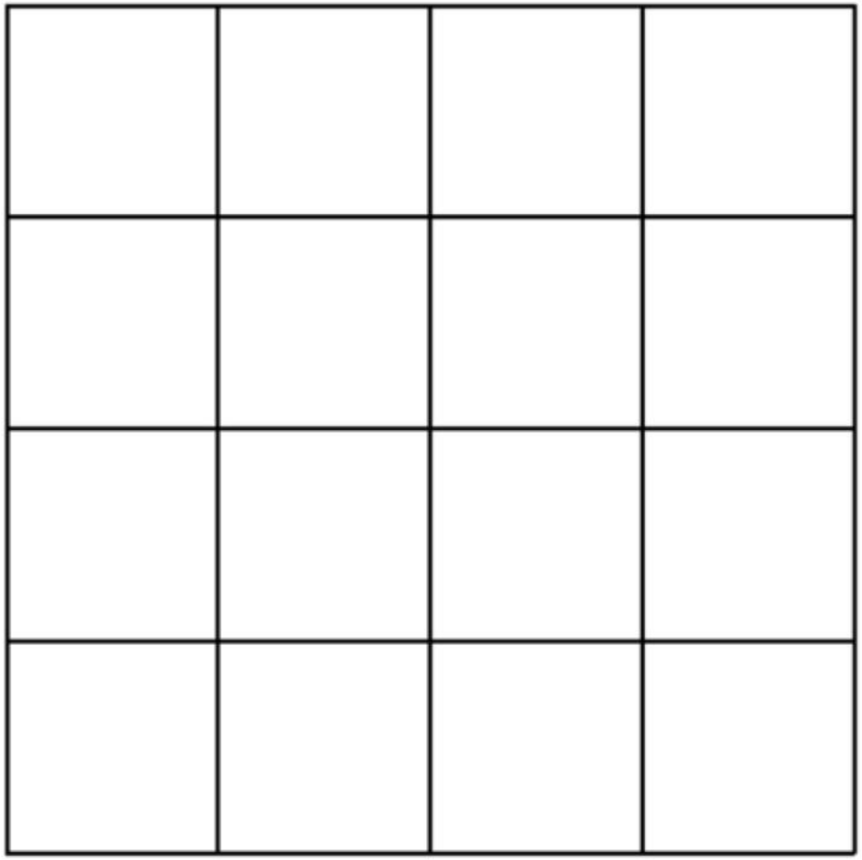
$$\begin{aligned} U_0 &= e^{\mathrm{i}kr}, \\ V_0 &= e^{\mathrm{i}kr}(-\mathrm{i}\omega) \end{aligned}$$

We define the error as the difference between the exact and numerical solution using the following error norm

$$\text{Error} = \frac{\left\| E - \widetilde{E} \right\|_{\mathrm{L}^p(\Omega)}}{\left\| \widetilde{E} \right\|_{\mathrm{L}^p(\Omega)}}$$

5.1 Example 1

The computational domain $\Omega = [0.1, 1.1] \times [0.1, 1.1]$ is meshed using 4-noded bilinear elements. The total number of elements is 16 with 25 nodes. The same mesh is retained for different wave numbers considered. The analytical solution of the problem is imposed on the domain boundary to eliminate the error coming from artificial boundary conditions. As mentioned earlier it is not possible to keep the same mesh if you change the wavenumber for the same domain in the standard FEM.

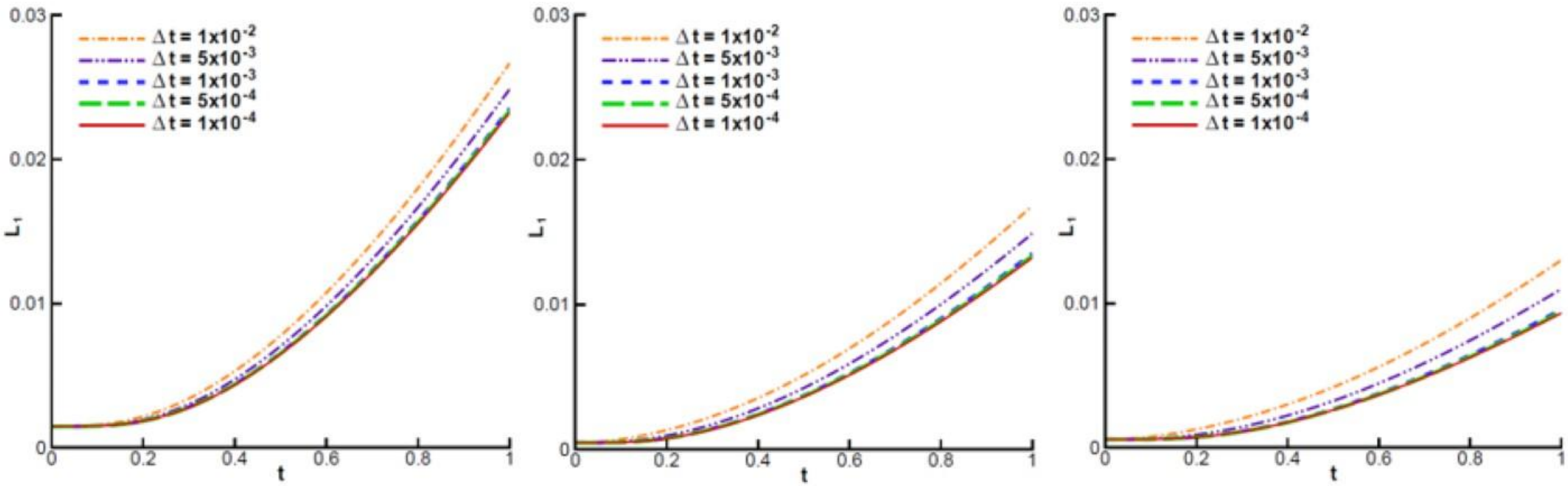


5.2 Example 1

Convergence study:

The plots show the convergence for smaller time steps for different wavenumbers.
The error consistently improve for smaller time steps and always converges.

$k = 8\pi,\ Q = 13$ | $k = 14\pi,\ Q = 23$ | $k = 20\pi\ Q = 31$

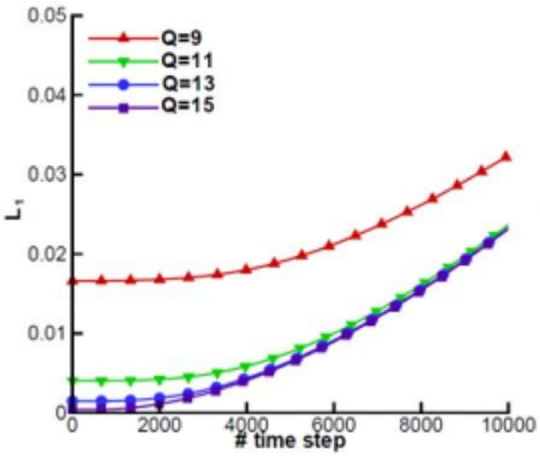


5.3 Example 1

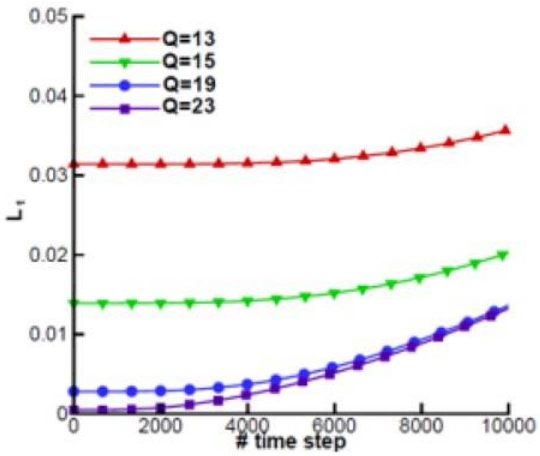
Convergence study:

The plots show the convergence for increasing the number of enrichment functions and for different wavenumbers. The error consistently improve for more enrichment functions and always converges. The time step is fixed at $\Delta t = 1.0 \times 10^{-04}$ which is the converged time step in the previous study.

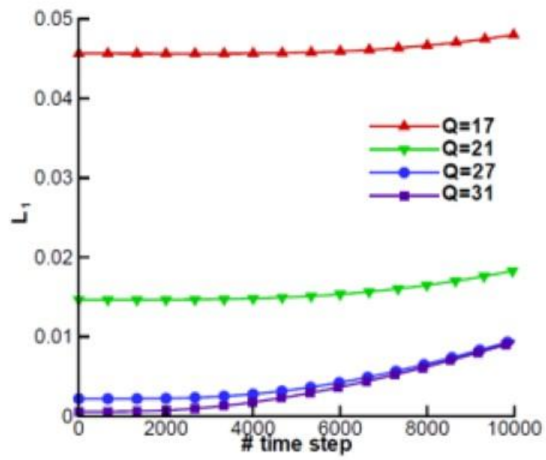
$k = 8\pi$



$k = 14\pi$



$k = 20\pi$

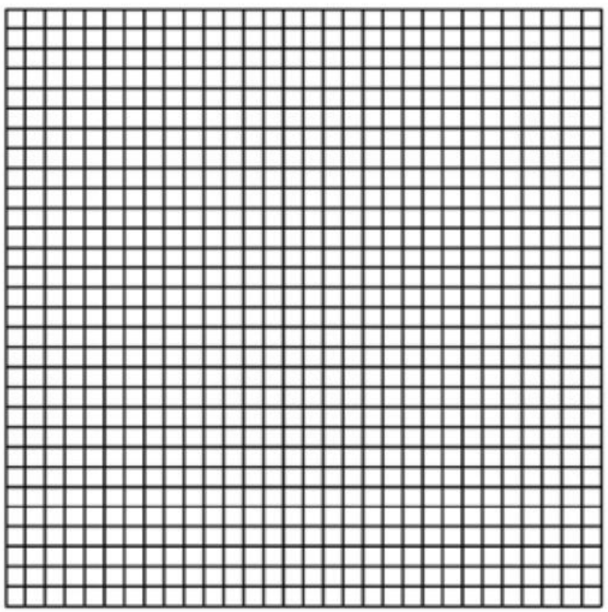


5.4 Example 1

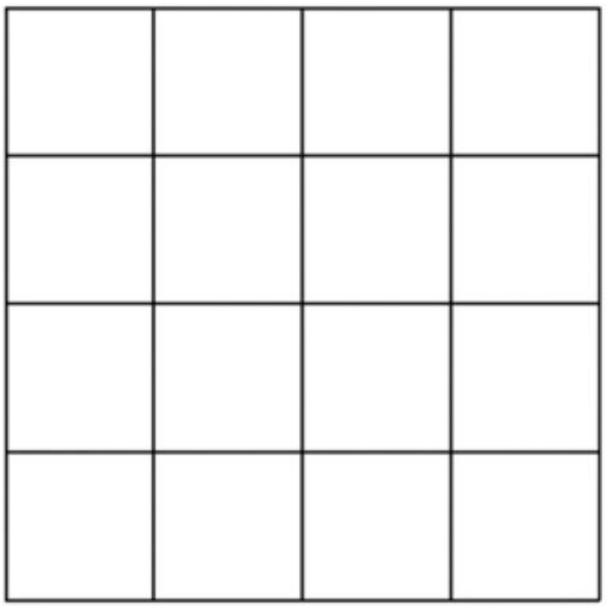
Comparison with the standard FEM:

Next we compare the PUFEM solution to the standard FEM solution. The problem is solved for $\Delta t = 1.0 \times 10^{-4}$ and $k = 6\pi$.

We consider two PUFEM solutions each with a different number of enrichment functions but the same mesh



FEM $N_{dof} = 961$

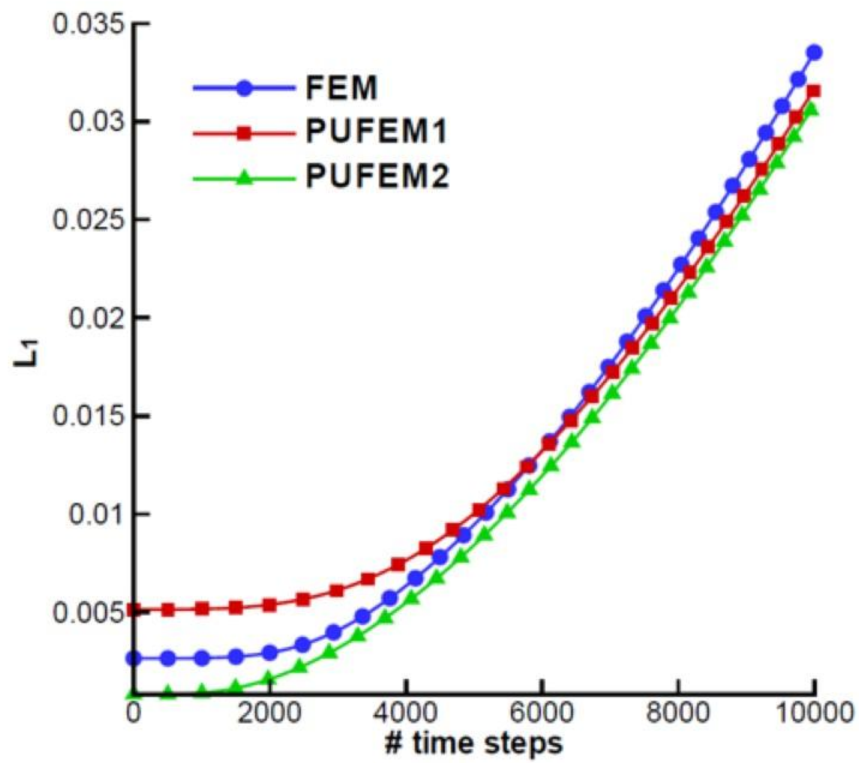


PUFEM1 $Q = 9$ $N_{dof} = 225$

PUFEM2 $Q = 11$ $N_{dof} = 275$

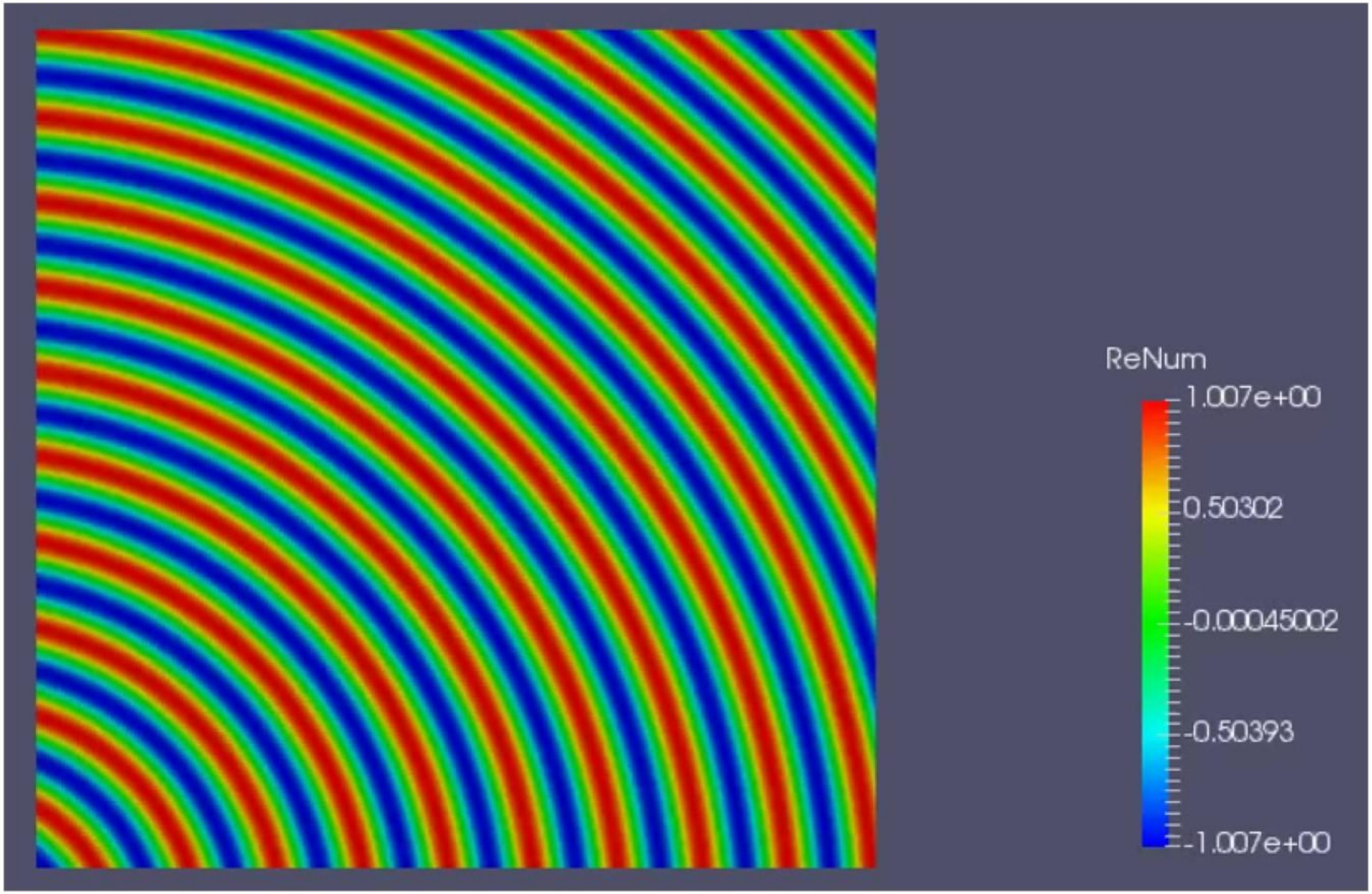
5.5 Example 1

At the first time step the FEM solution error is smaller than PUFEM1 and larger than PUFEM2. However, as the solution progresses in time the PUFEM1 and PUFEM2 solution accumulates error at a smaller rate in time compared to the FEM which leads to better error with both than with the FEM



5.6 Example 1

The animation is created for $k = 20\pi \quad \Delta t = 1.0 \times 10^{-3} \; Q = 26$



6.0 Example 2

In the second test example we consider a problem with the following analytical solution. The problem starts with a constant solution and then a circular wave is introduced into the domain using a propagator function. The exact solution is given by

$$\widetilde{E}(t,x,y) = Ae^{\mathrm{i}wf_L(t,x,y)}$$

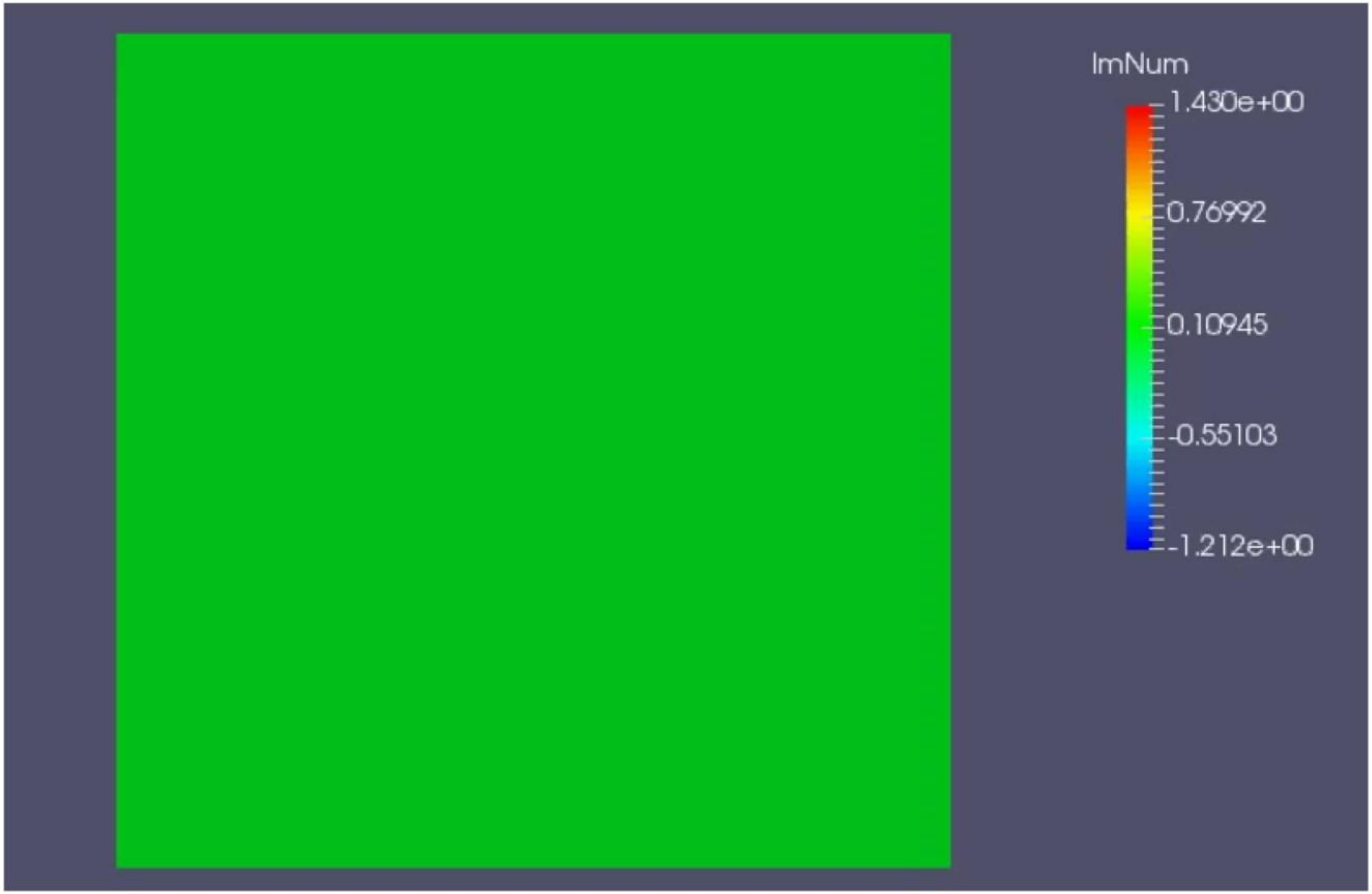
While the propagator function is defined by

$$f_L(p) = \frac{1}{1+a}\left(\operatorname{erf}\left(\frac{p-p_0}{b}\right)(p-p_0) + ap + \frac{b}{\sqrt{\pi}}e^{-\frac{(p-p_0)^2}{b^2}}\right)$$

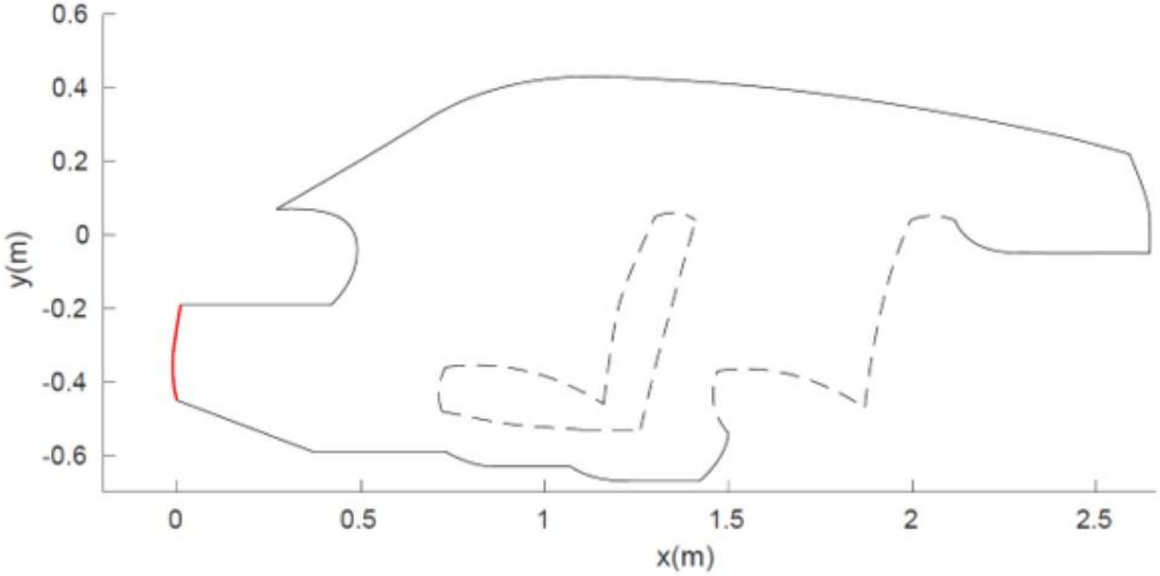
The problem is again considered over the unit square domain and the initial conditions are defined based on the exact solution. The solution is also imposed on the domain boundary through the boundary conditions to avoid error resulting from artificial boundary conditions.

6.1 Example 2

The wave propagator animation created for the considered parameters



7.0 Example 3



$$\int_{\Omega} \left(\nabla u \overline{\nabla v} - k^2 u \bar{v}\right) d\Omega + \int_{\Gamma_Z} Z u \bar{v} = \int_{\Gamma_N} g_N \bar{v}$$

$$\rho_{air} = 1 \text{ kg m}^{-3}$$

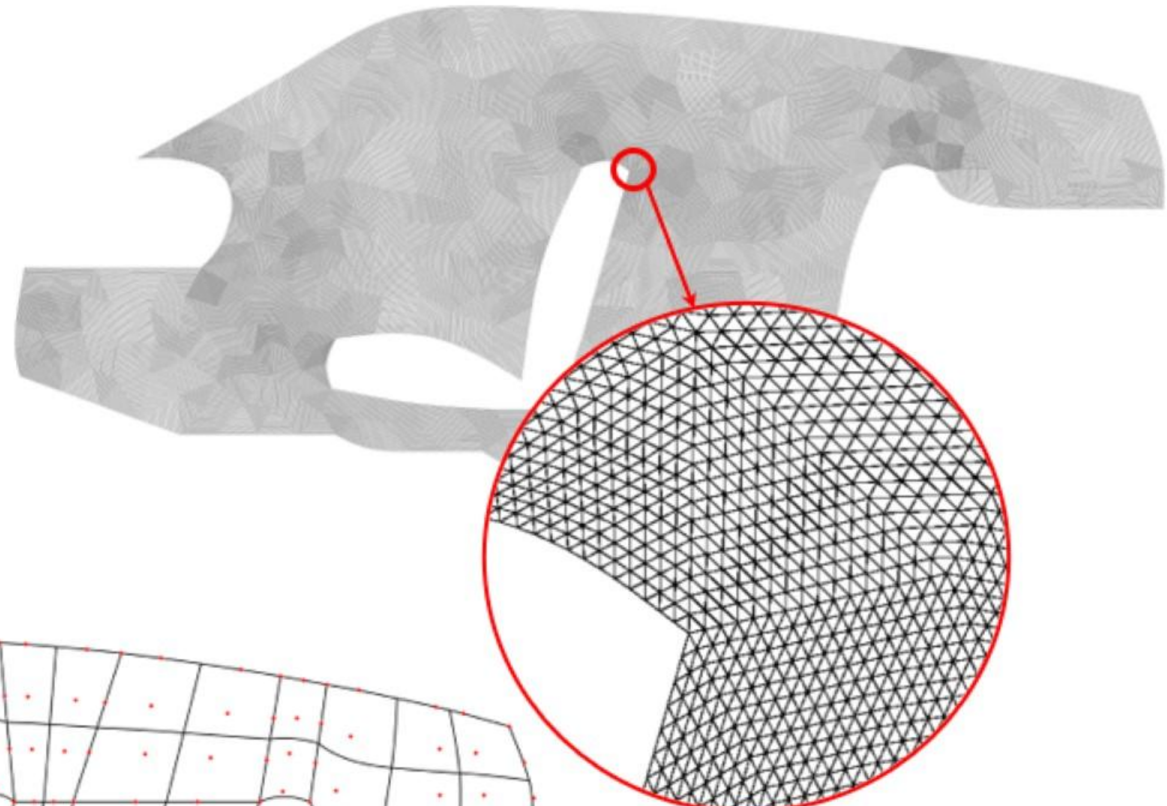
$$v_n = 1 \text{ m s}^{-1}$$

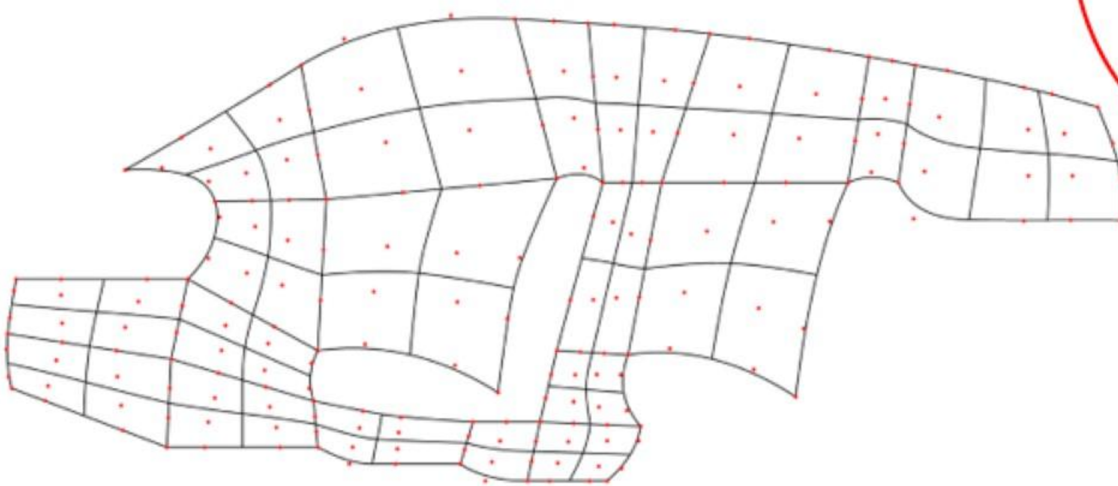
$$Z_0 = 2000 \text{ ryal}$$

$$\frac{\partial u}{\partial n} = -2\pi \mathrm{i} f \rho_{air} v_n \text{ on } \Gamma_N$$

$$\frac{\partial u}{\partial n} = -2\pi \mathrm{i} f \rho_{air} \frac{u}{Z_0} \text{ on } \Gamma_Z$$

7.1 Example 3

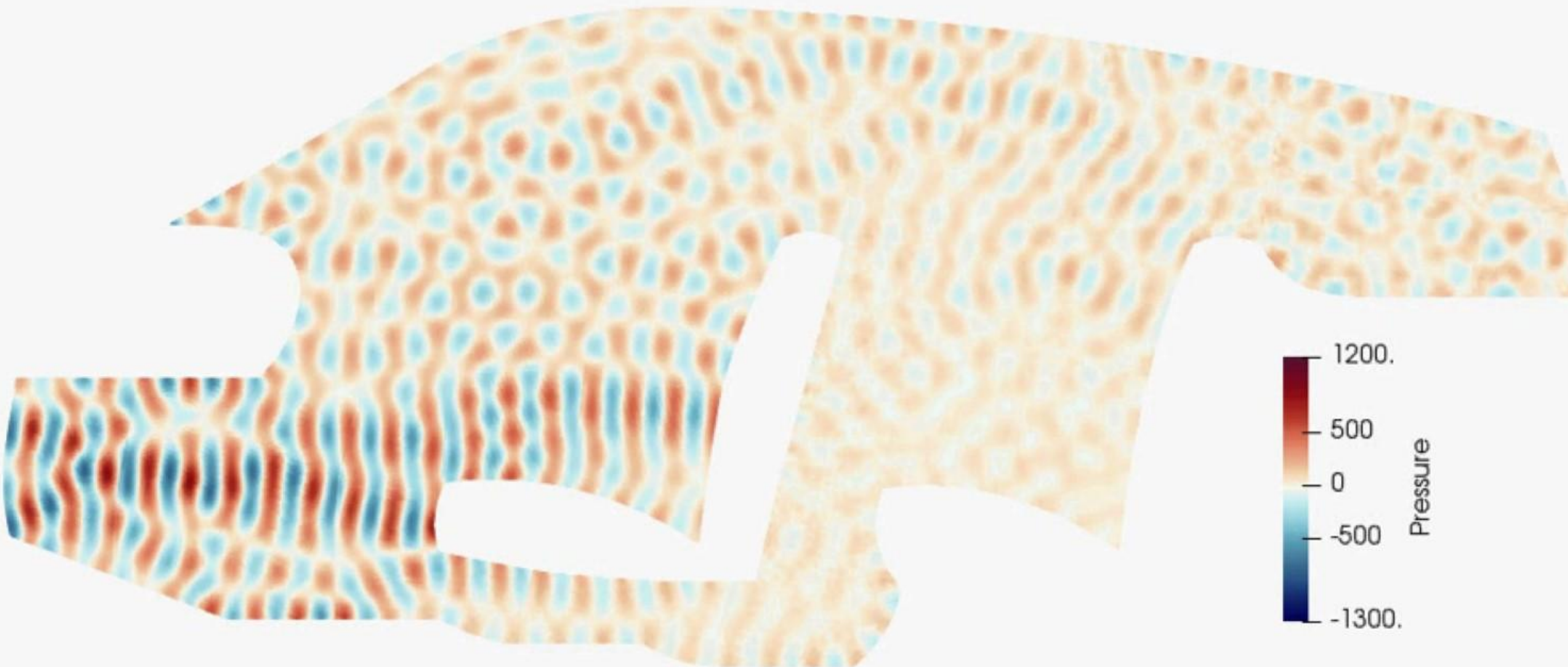




7.2 Example 3

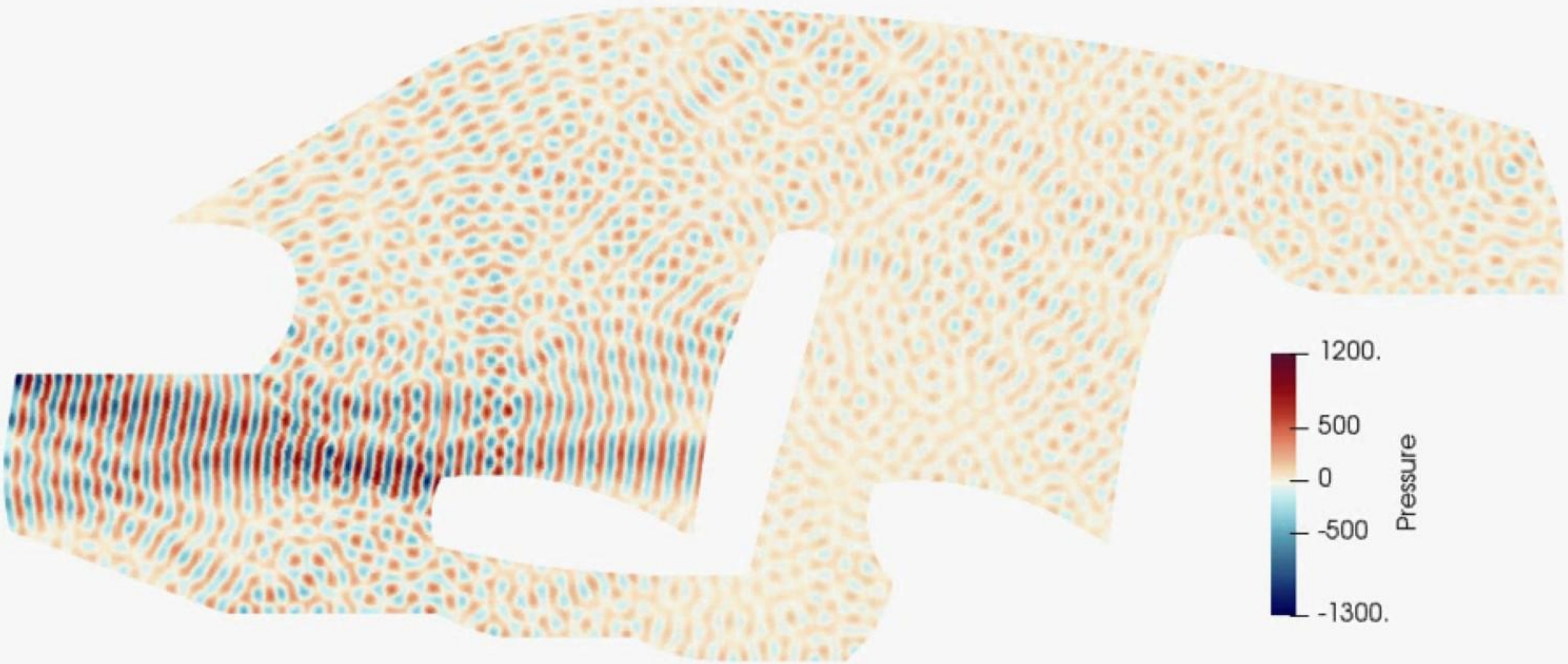
$$f = 0.5 \text{ kHz}$$

7.3 Example 3



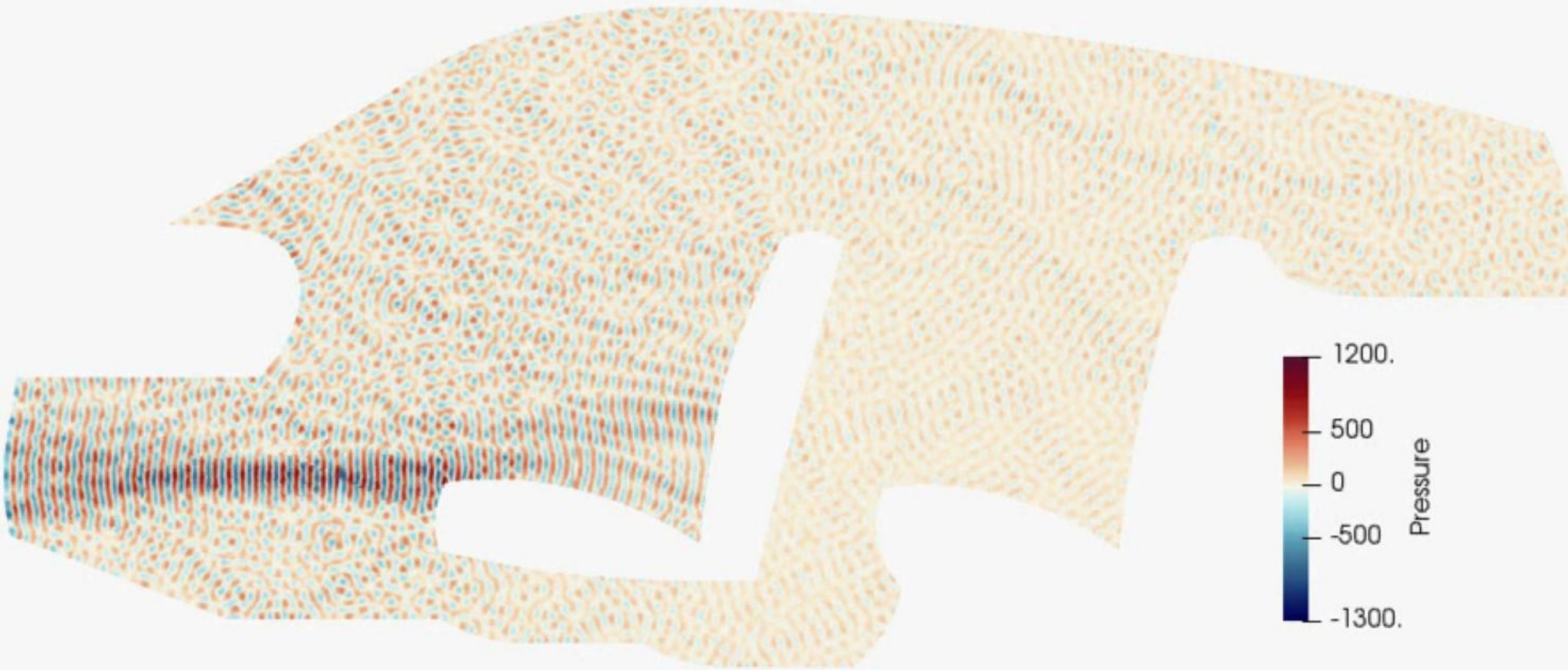
$f = 5$ kHz

7.4 Example 3



$f = 10$ kHz

7.5 Example 4



$f = 15 \text{ kHz}$

7.6 Example 3

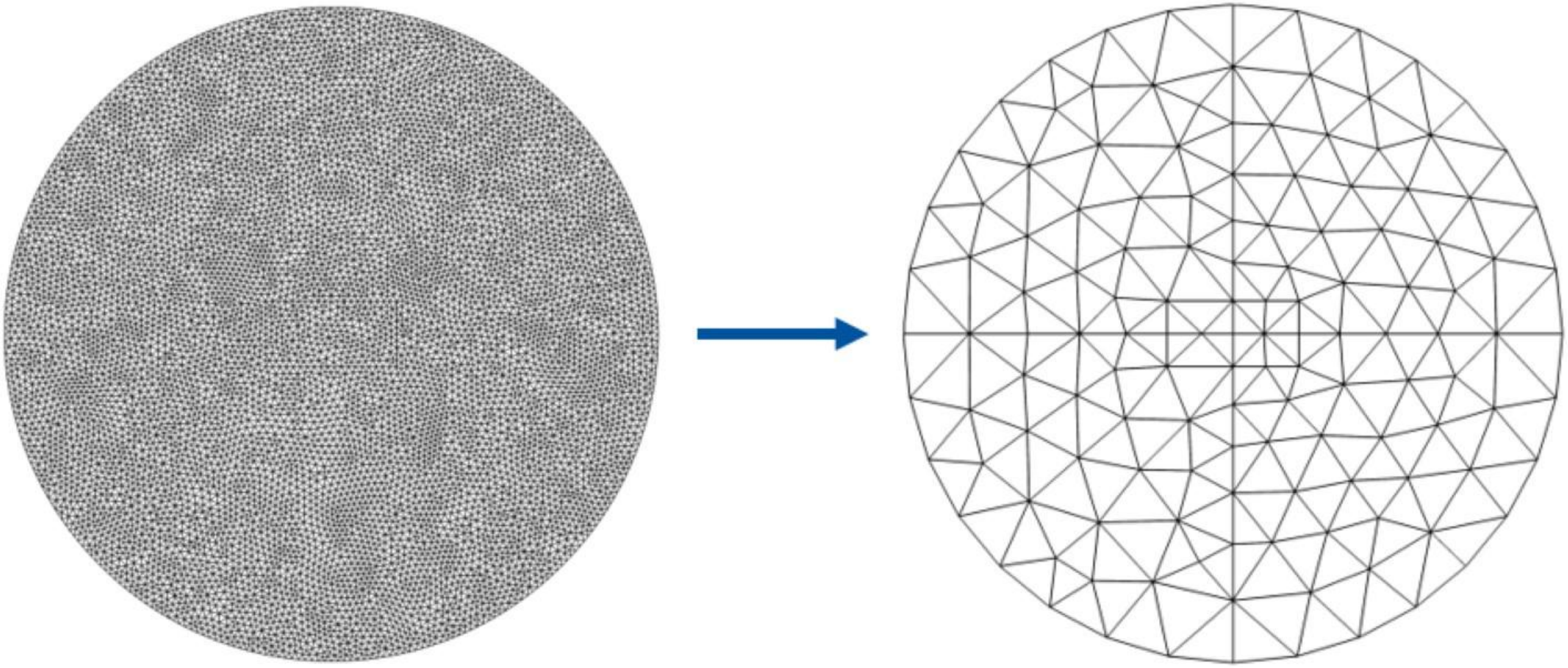
$f = 20 \text{ kHz}$

Transient heat transfer

8.0 Challenges




9.0 Objective



Reduce the computational costs

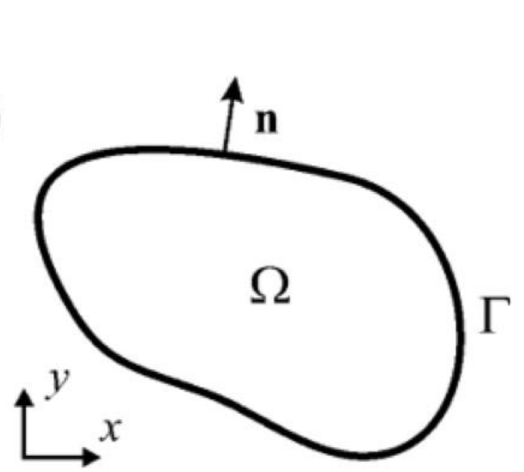
10.0 Non-linear heat diffusion

Problem definition:

$$\rho(t,\mathbf{x},\Theta)\,c(t,\mathbf{x},\Theta)\,\frac{\partial\Theta}{\partial t} - \nabla\cdot\Big(\kappa(t,\mathbf{x},\Theta)\,\nabla\Theta\Big) = f(t,\mathbf{x},\Theta)$$

$$\kappa(t,\hat{\mathbf{x}},\Theta)\,\frac{\partial\Theta}{\partial\mathbf{n}} + \Theta(t,\hat{\mathbf{x}}) = g(t,\hat{\mathbf{x}},\Theta)$$

$$\Theta(0,\mathbf{x}) = \Theta_0(\mathbf{x})$$



Using the first order Backward Euler scheme we get:

$$\rho^n(\mathbf{x},\Theta^n)\,c^n(\mathbf{x},\Theta^n)\,\Theta^{n+1} - \Delta t\nabla\cdot\Big(\kappa^n(\mathbf{x},\Theta^n)\,\nabla\Theta^{n+1}\Big) = F \qquad (0,T]$$

$$F = \Delta t f^{n+1}(\mathbf{x},\Theta^n) + \rho^n(\mathbf{x},\Theta^n)\,c^n(\mathbf{x},\Theta^n)\,\Theta^n$$

Using the divergence theorem and substituting the boundary condition the following weak formulation of the problem is obtained:

$$\int_\Omega\Big(\rho^n(\mathbf{x},\Theta^n)\,c^n(\mathbf{x},\Theta^n)\,\phi\Theta^{n+1} + \Delta t\kappa^n(\mathbf{x},\Theta^n)\,\nabla\phi\cdot\nabla\Theta^{n+1}\Big)\,d\Omega +$$

$$\oint_\Gamma \Delta t\Big(\Theta^{n+1} - g^{n+1}(\mathbf{x},\Theta^n)\Big)\phi\,d\Gamma = \int_\Omega F\phi\,d\Omega$$

11.0 Partition of unity method

Following the standard finite element approximation we evaluate the temperature at the nodes and approximate the solution in between the nodes using polynomial (often linear) interpolation

$$\Theta_h^n = \sum_{j=1}^{\#\text{ nodes}} C_j^n N_j(\mathbf{x})$$

Alternatively using the partition of unity method we expand the unknown temperature at the nodes into a set of exponential functions:

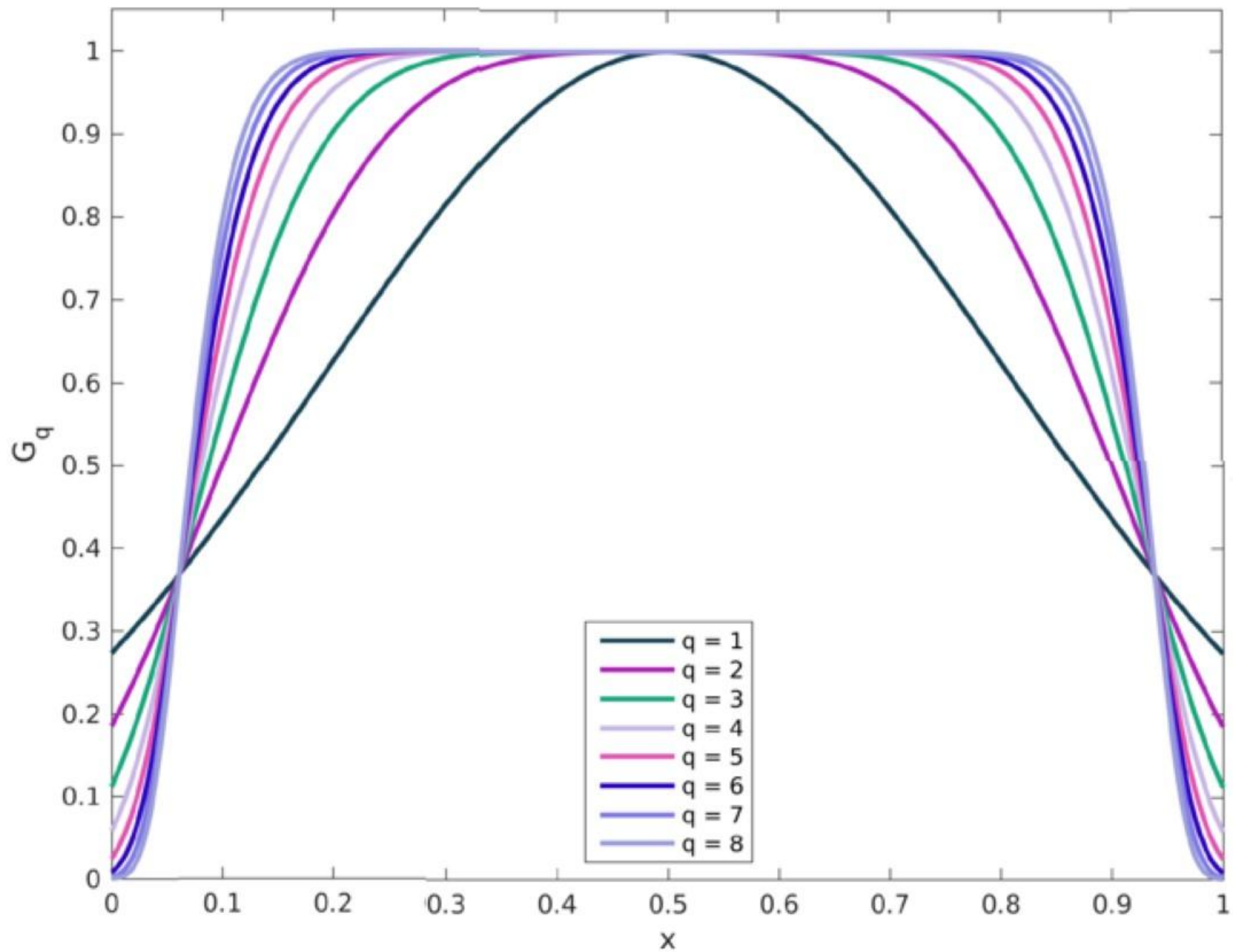
$$\Theta_h^n = \sum_{j=1}^{\#\text{ nodes}} \sum_{q=1}^{Q} C_{j,q}^n N_j(\mathbf{x}) G_q(\mathbf{x})$$

with

$$G_q(\mathbf{x}) = \frac{\exp\left(-\left(\frac{R_0}{C}\right)^q\right) - \exp\left(-\left(\frac{R_c}{C}\right)^q\right)}{1 - \exp\left(-\left(\frac{R_c}{C}\right)^q\right)}$$

12.0 Enrichment

The Gaussian enrichment functions have certain difficulties linked to them. This can be seen in the following plot:



13.0 Example 1 (3D)

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$\Omega = [-2,2] \times [-2,2] \times [-2,2]$ $\qquad \kappa = 0.1 \quad \rho = c = 1.0$

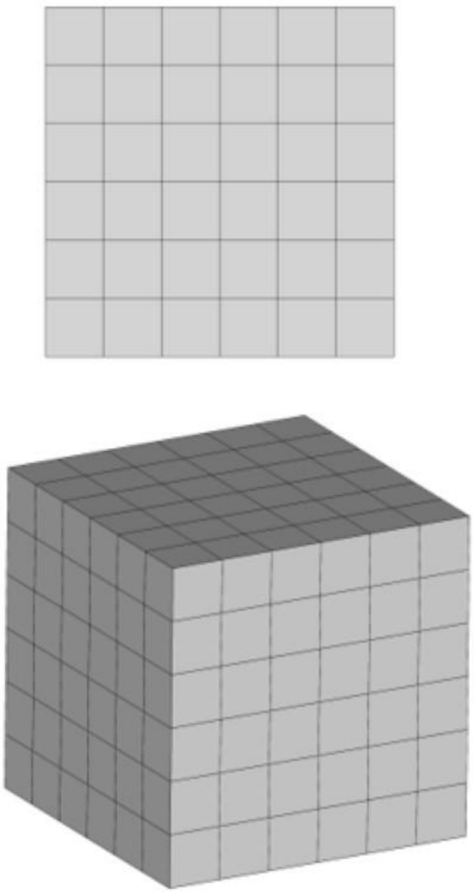
$$\Theta(t,x,y,z) = x^{20}y^{20}z^{20}(2-x)^{20}(2-y)^{20}(2-z)^{20}(1-e^{-\kappa t})$$

The problem is solved for an increased number of enrichment functions using iterative (CMRH[1], GMRES) and direct (SVD and variations of Gaussian Elimination) solvers.

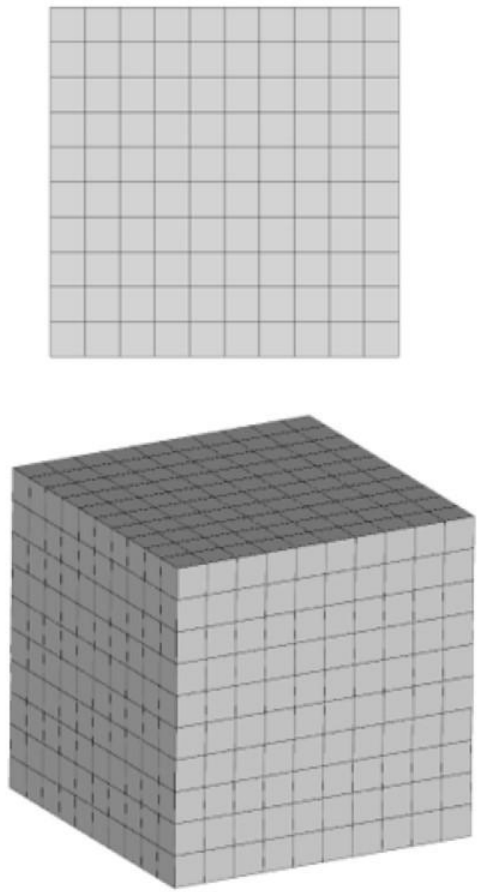
	FE1	FE2	FE3	FE4
# Nodes/Degrees of freedom	1331	9261	17576	29791
# Elements	1000	8000	15625	27000

	PU2	PU3	PU4	PU5	PU6
# Enrichment funcctions	2	3	4	5	6
# Degrees of freedom	686	1029	1372	1715	2058

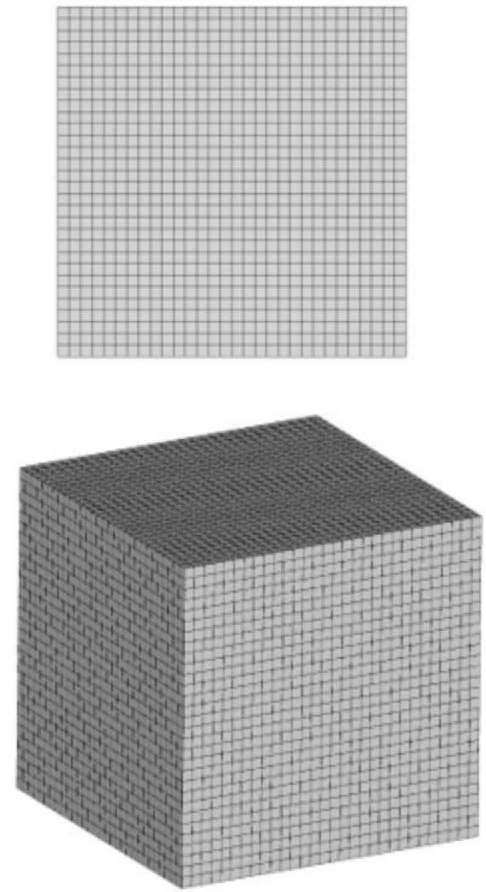
13.1 Example 1 (3D)



PUFEM
216e & 343n



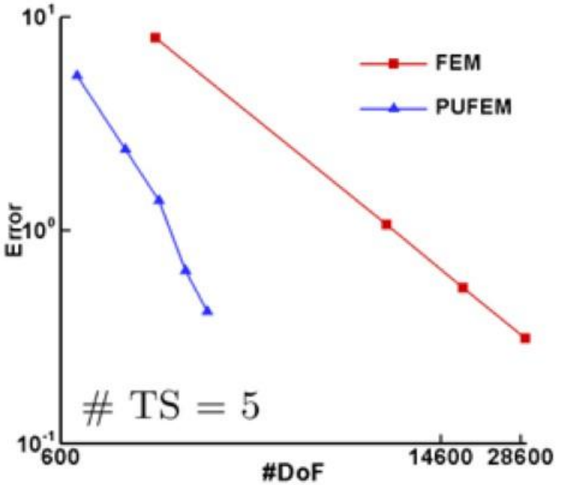
FEM
1000e & 1331n

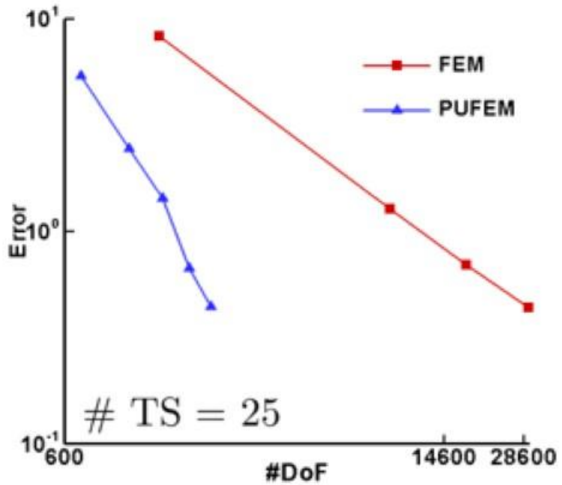


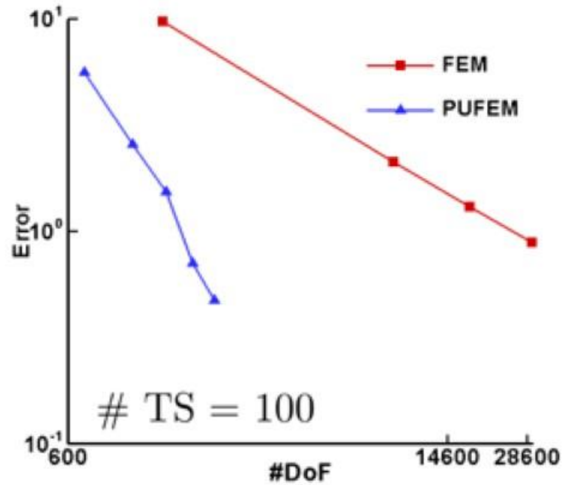
FEM
27000e & 29791n

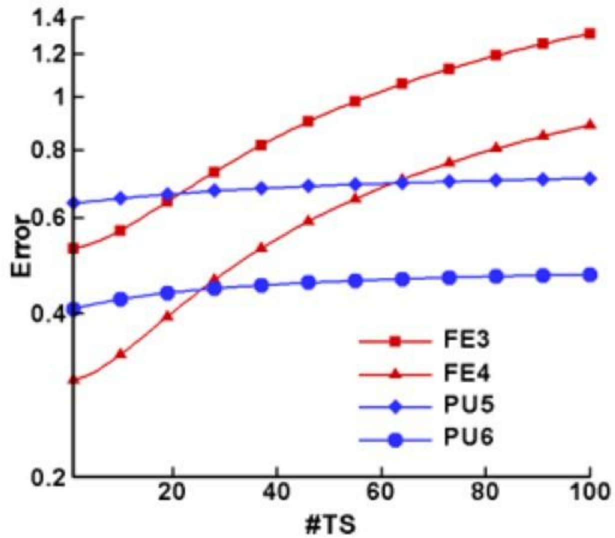
13.2 Example 1 (3D)

$\Delta t = 0.001$



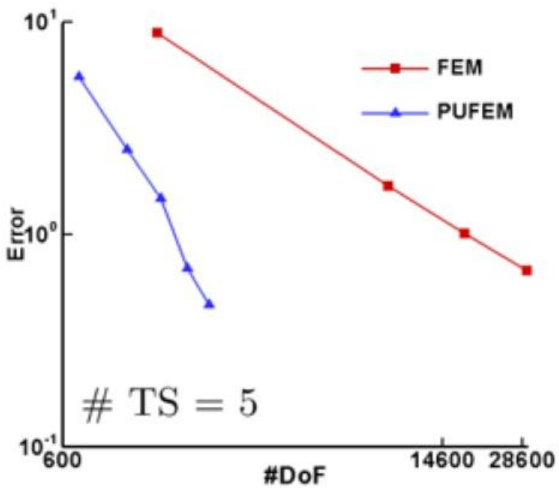


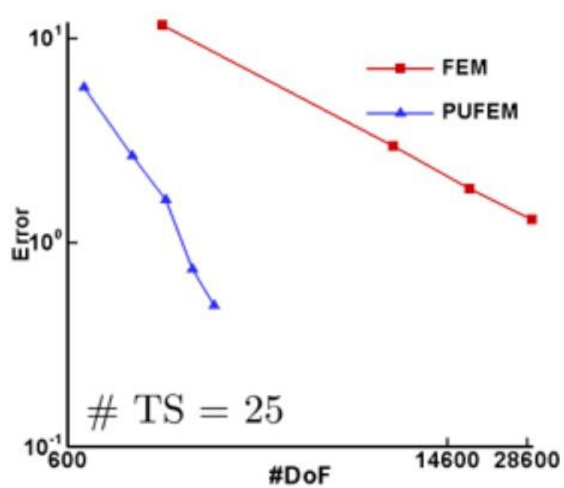


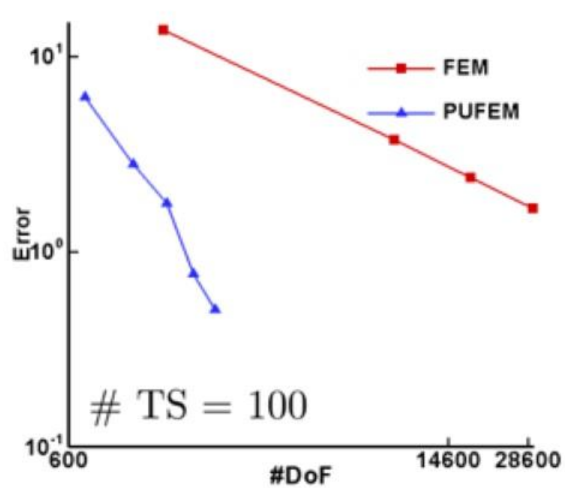


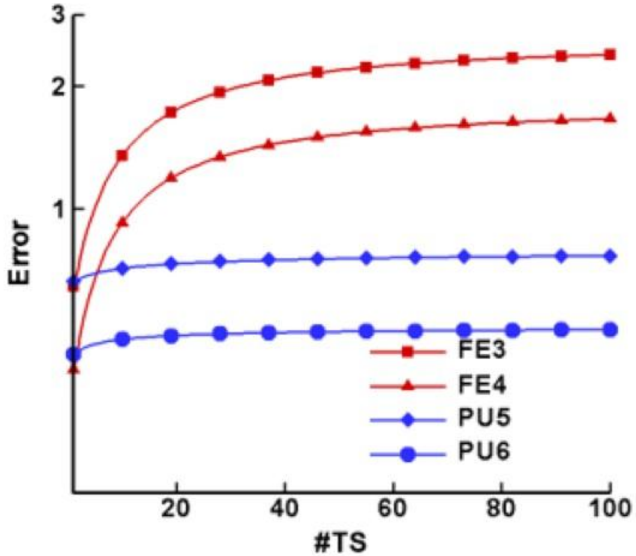
13.3 Example 1 (3D)

$\Delta t = 0.01$







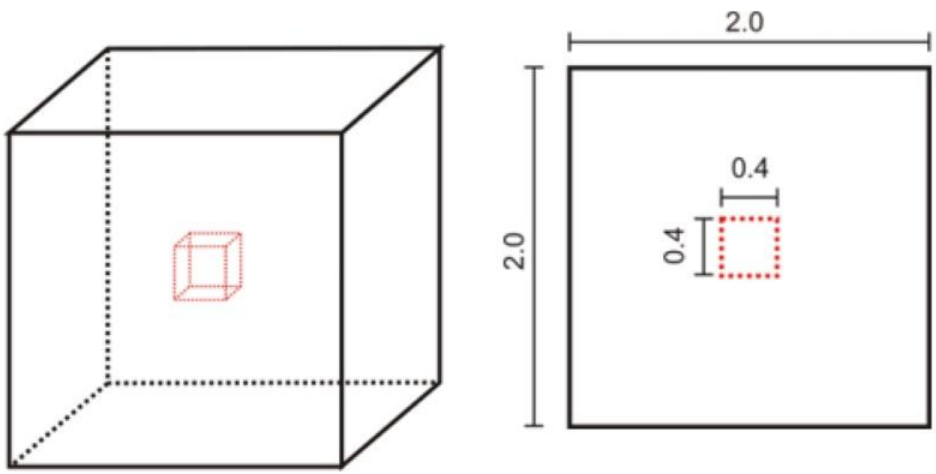


13.4 Example 1 (3D)

		CPU time (s)	
	time step	build/rebuild	solve/resolve
PU2	1st	217.86	0.03
	2nd	0.66	0.00
PU3	1st	218.73	0.05
	2nd	0.70	0.00
PU4	1st	219.09	0.13
	2nd	0.78	0.00
PU5	1st	220.41	0.25
	2nd	1.05	0.02
PU6	1st	221.35	0.39
	2nd	1.09	0.02

		CPU time (s)	
	time step	build/rebuild	solve/resolve
FE1	1st	1020.98	0.05
	2nd	1.75	0.00
FE2	1st	8118.54	3.62
	2nd	12.83	0.05
FE3	1st	15770.16	15.83
	2nd	26.66	0.14
FE4	1st	27407.33	54.35
	2nd	44.23	0.37

14.0 Example 2 (3D)

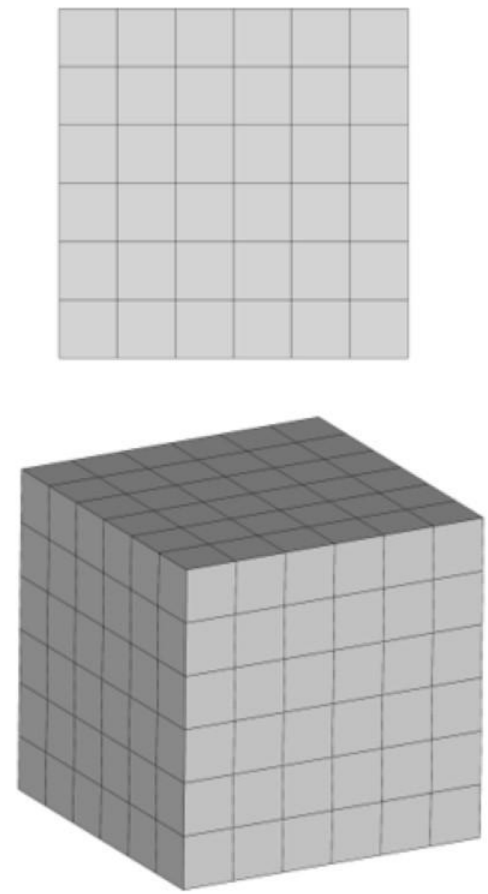


$$\Omega = [-2,2] \times [-2,2] \times [-2,2]$$

$$\Delta t = 0.01 \quad \kappa = 0.1 \quad \rho = c = 1.0$$

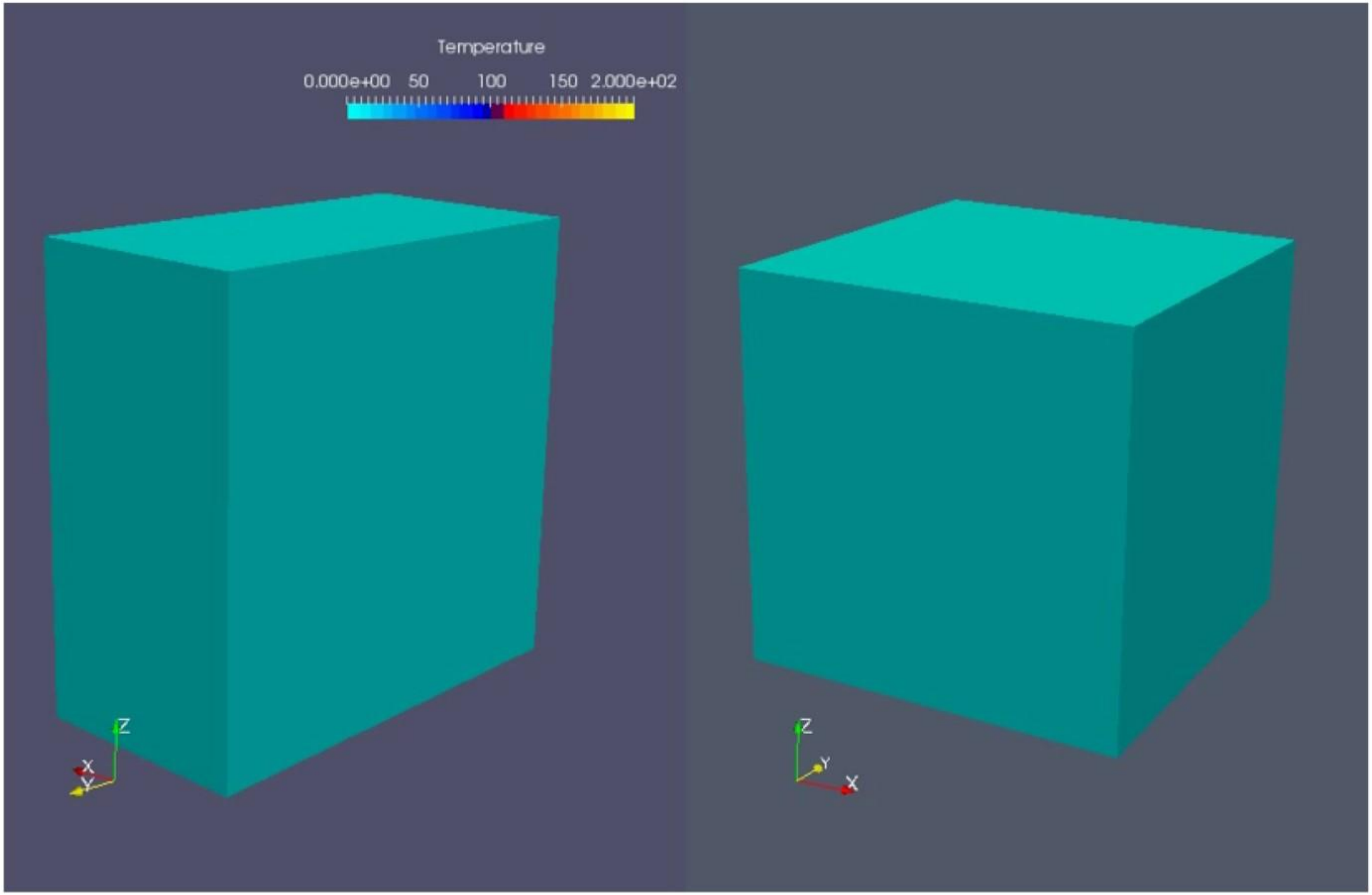
$$\Theta_0 = 0 \quad \Theta_b = 0 \quad \Theta_c = 400$$

$$Q = 5 \qquad DoFs = 1372$$

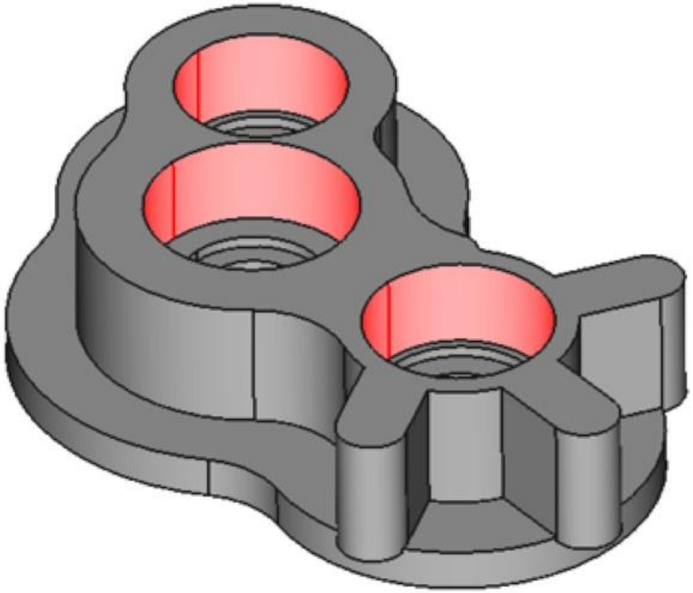


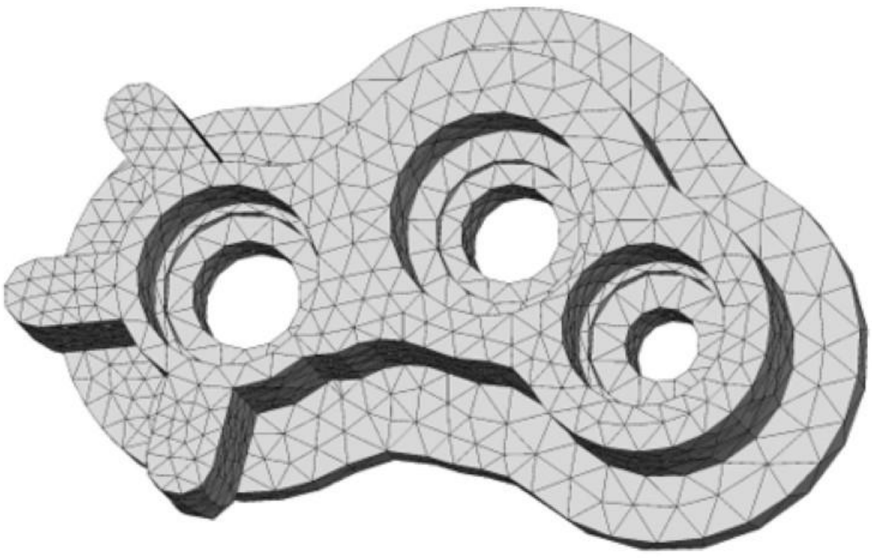
PUFEM
216e & 343n

14.1 Example 2 (3D)



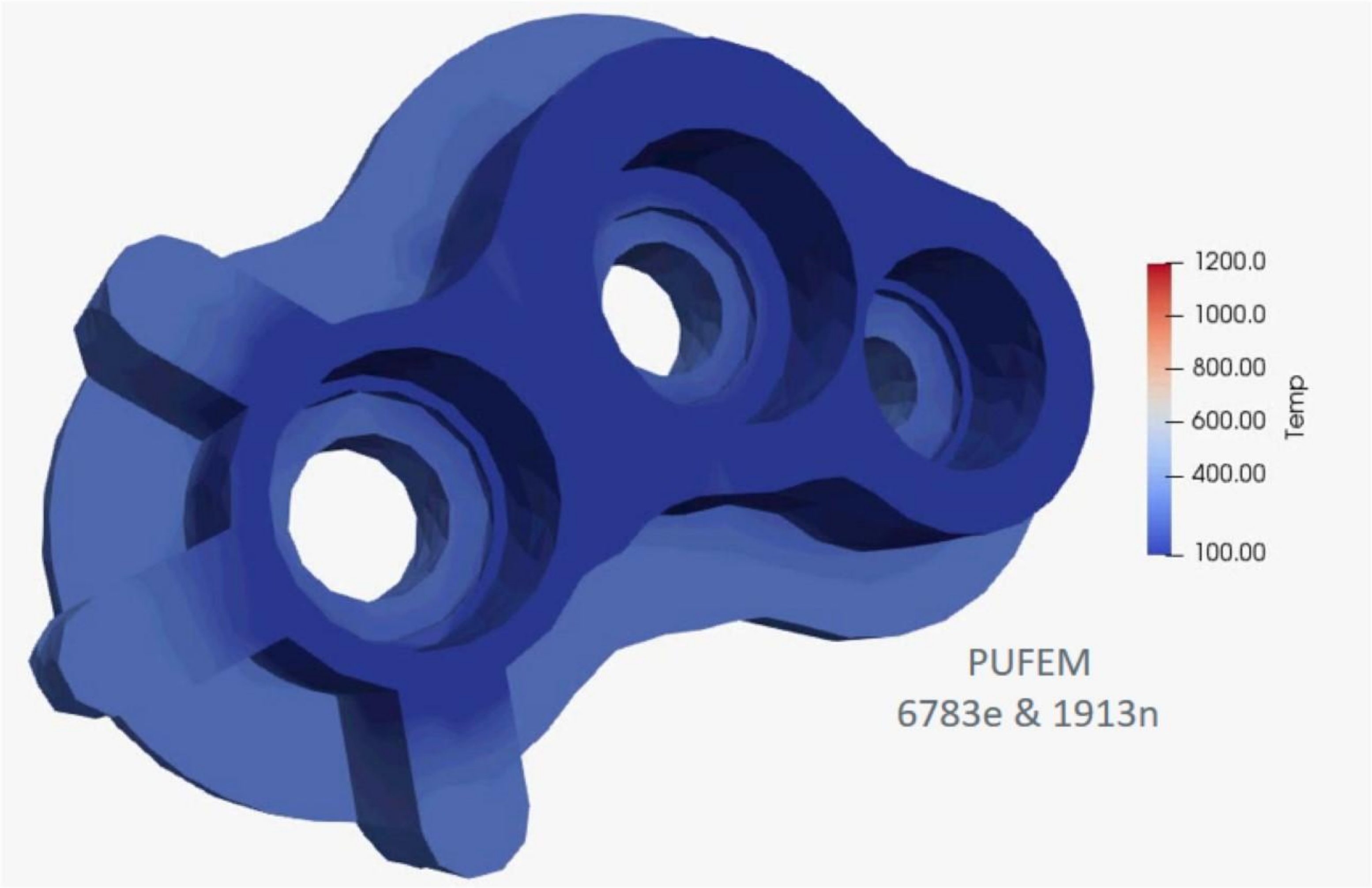
15.0 Example 3 (3D)



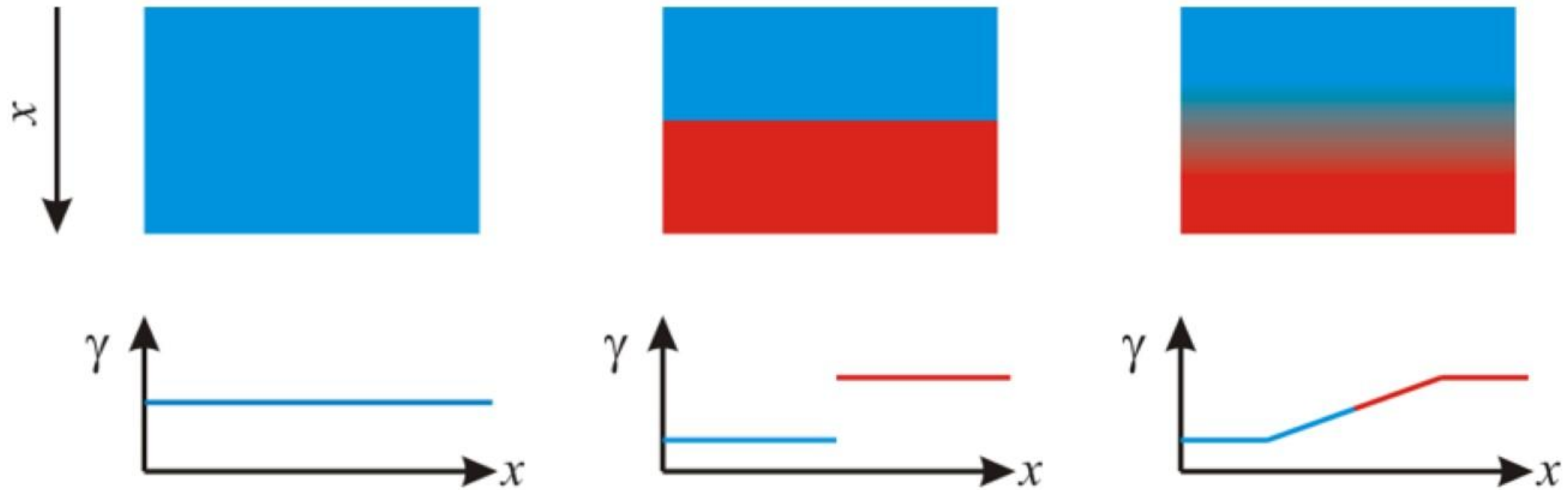


PUFEM
6783e & 1913n

15.1 Example 3 (3D)



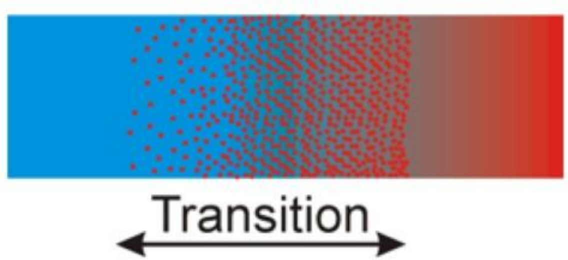
16.0 Functionally graded materials



Homogeneous

Composite

Functionally Graded Material (FGM)



17.0 Example 4 (FGM)

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FGM of Zirconium dioxide and a Titanium alloy:

$$f(x,y) = 5 \times 10^6 \left(1 + \sin(10\pi x)\sin(10\pi y)\right)$$
$$g(t,\hat{\mathbf{x}}) = 0\,K \qquad \Delta t = 1\,s \qquad \Theta_0 = 300\,K$$

Zirconium dioxide (ZrO2) material properties:

$$\begin{aligned}
\kappa(\Theta) &= 1.71 + 2.1 \times 10^{-4}\Theta + 1.16 \times 10^{-7}\Theta^2, \\
c(\Theta) &= 2.74 \times 10^2 + 7.95 \times 10^{-1}\Theta - 6.19 \times 10^{-4}\Theta^2 + 1.71 \times 10^{-7}\Theta^3 \\
\alpha(\Theta) &= 1.331 \times 10^{-5} - 1.89 \times 10^{-8}\Theta + 1.27 \times 10^{-11}\Theta^2, \\
\rho(\Theta) &= 3657/\left(1 + \alpha(\Theta - 300)\right)^3,
\end{aligned}$$

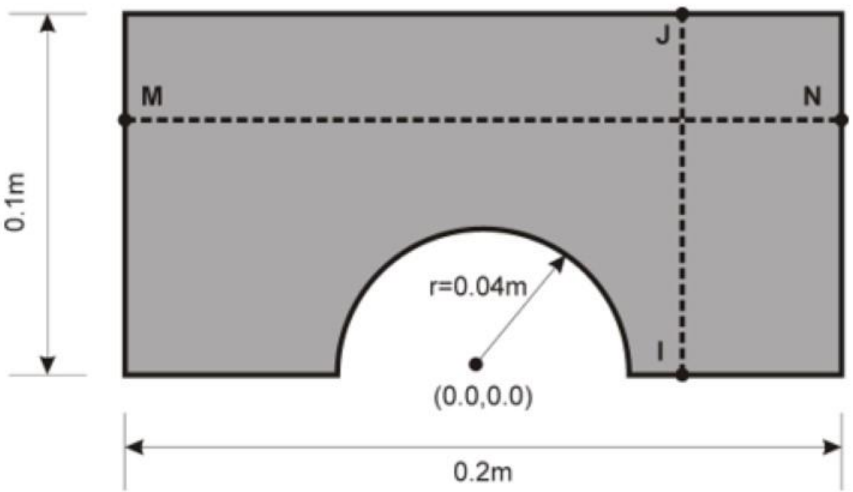
Titanium alloy (Ti-6Al-4v) material properties:

$$\begin{aligned}
k(\Theta) &= 1.1 + 1.7 \times 10^{-2}\Theta, \\
c(\Theta) &= 3.5 \times 10^2 + 8.78 \times 10^{-1}\Theta - 9.74 \times 10^{-4}\Theta^2 + 4.43 \times 10^{-7}\Theta^3 \\
\alpha(\Theta) &= 7.43 \times 10^{-6} + 5.56 \times 10^{-9}\Theta - 2.69 \times 10^{-12}\Theta^2, \\
\rho(\Theta) &= 4420/\left(1 + \alpha(\Theta - 300)\right)^3,
\end{aligned}$$

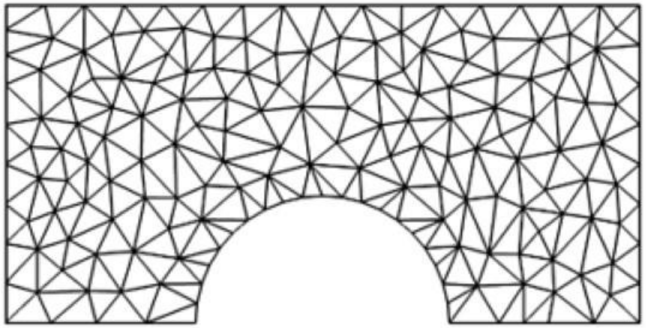
Mixture rule is volume fractions of the material are changing linearly

$$p = p_1\nu_1 + p_2\nu_2$$

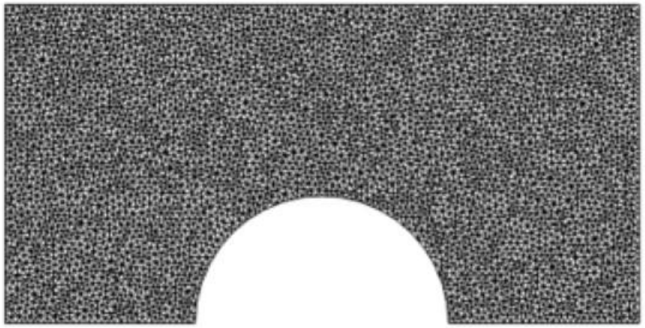
17.1 Example 4 (FGM)



Problem configuration

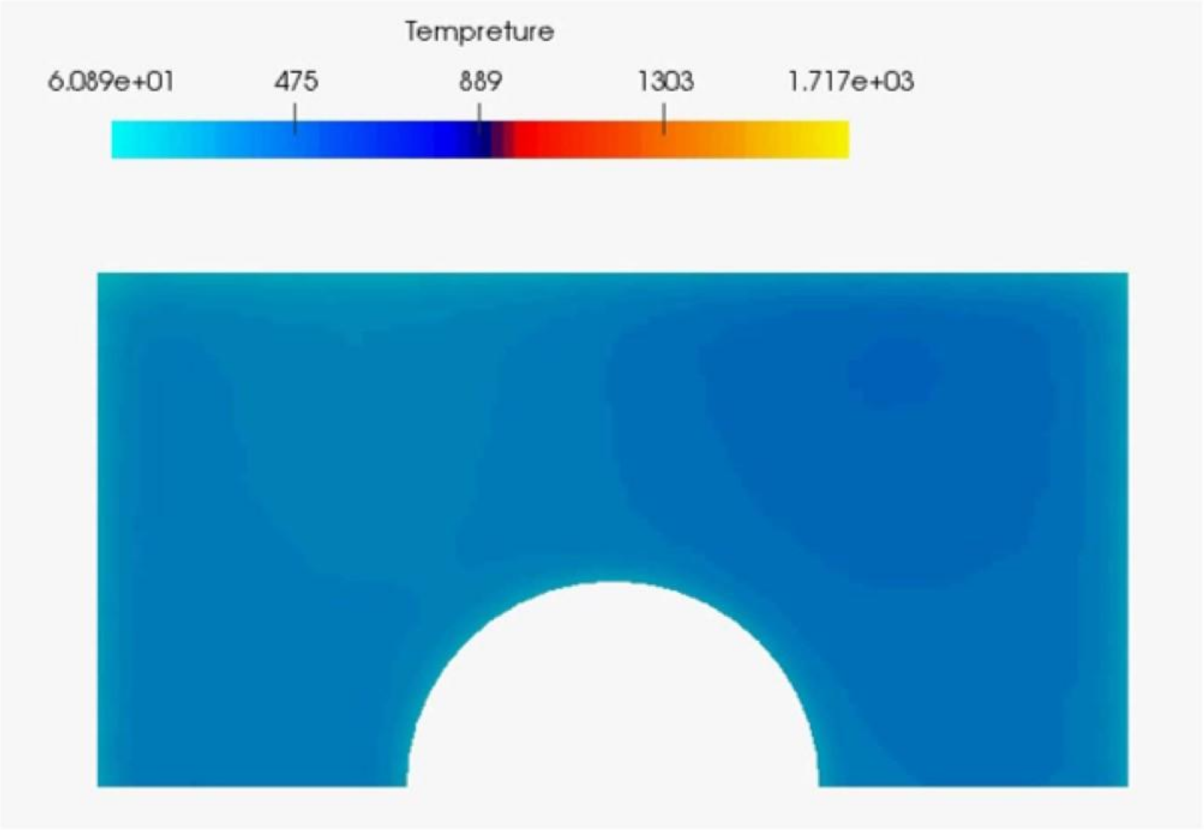


Mesh 1 (332e, 201n)



Mesh 2 (10013e, 5194n)

17.2 Example 4 (FGM)



18.0 ill-conditioning issue

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A major problem in the partition of unity method is related to the ill-conditioned linear system that can be produced when using a large number of enrichment function. We will discuss this issue in the heat transfer problem but a similar discussion also apply to the wave problem.
The weak formulation for heat transfer we have used before is:

$$\int_{\Omega}\Big(D\Delta t\nabla\varphi\cdot\nabla u^{n+1}+\varphi u^{n+1}\Big)\,d\Omega+\oint_{\Gamma}\Delta t\Big(u^{n+1}-g^{n+1}\Big)\varphi\,d\Gamma=\int_{\Omega}\Big(u^{n}+\Delta t f^{n+1}\Big)\varphi\,d\Omega$$

Using the partition of unity method we approximate he solution using:

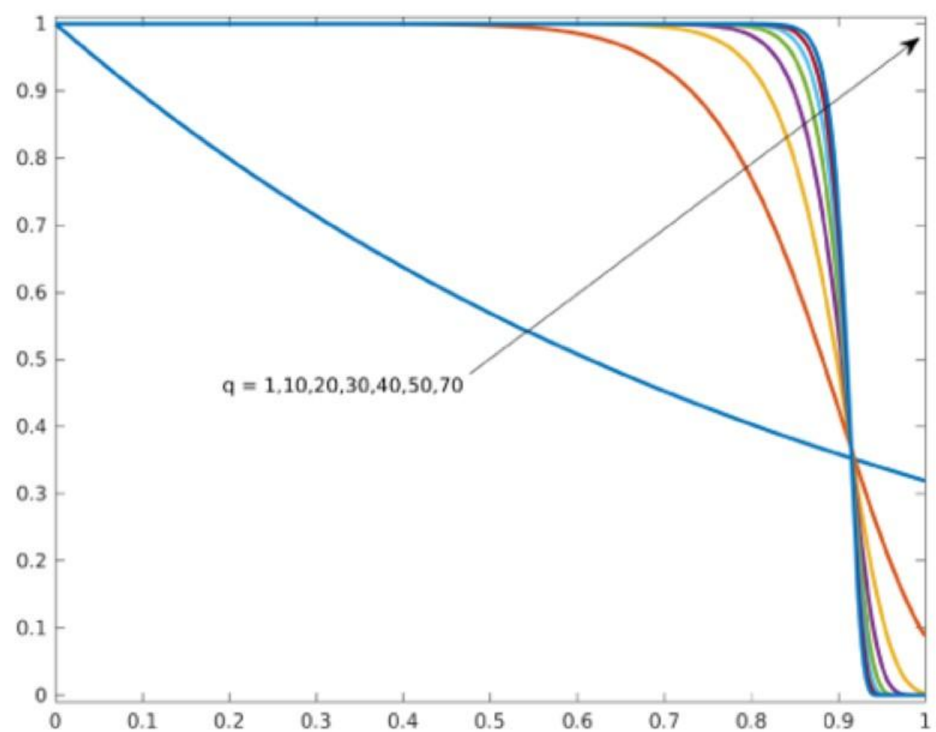
$$u_h^{n+1}(\xi)=\sum_{j=1}^{N}\sum_{q=1}^{Q}U_j^{q,n+1}\Phi_j G_q(\xi)$$

18.1 ill-conditioning issue

The enrichment function is then given in the following form

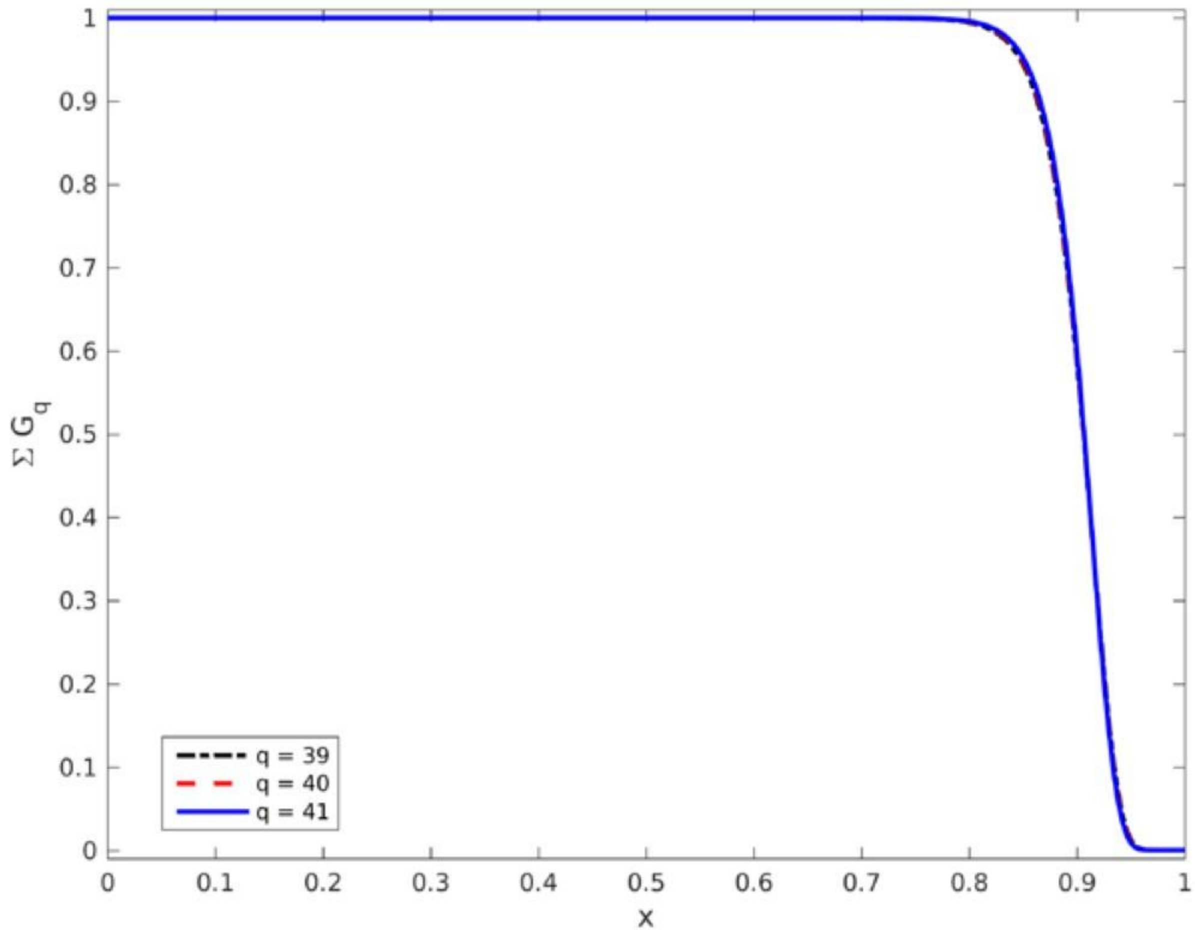
$$G_q(\xi) = \frac{\exp\left(-\left(\frac{r}{C}\right)^{m_q}\right) - \exp\left(-\left(\frac{R_c}{C}\right)^{m_q}\right)}{1 - \exp\left(-\left(\frac{R_c}{C}\right)^{m_q}\right)}, \qquad q = 1, 2, \ldots, Q$$

If we plot the enrichment function for different orders then we get



18.2 ill-conditioning issue

We can take a closer look we can see that as a higher order is considered the difference between one function and the other becomes negligible. Considering the machine precision the orders 39, 40 and 41 of the function would start to look very much the same.



23.0 Conclusion

- We used enriched finite elements to solve waves and heat diffusion problems.
- The achieved reduction is up to 95% of the number of degrees of freedom required with the standard finite element.
- The proposed approach uses time independent enrichment which significantly reduces the computational costs of the time stepping.
- This is done by decomposing the system at the first time-step and then reusing this decomposition at later time steps after updating the right-hand side.
- The approach used for the conduction problem in homogeneous and heterogeneous problem.
- One topic that must be discussed is the ill-conditioning issue.