Computational Rheology @IPC

17th OpenFOAM Workshop

# OFW17: Code verification through the method of manufactured solutions

B. Ramoa , R. Costa, F. Chinesta, J.M. Nóbrega

bruno.ramoa@dep.uminho.pt

Researcher @IPC-UMinho

http://www.ipc.uminho.pt/

https://crheo.org/

University of Minho School of Engineering

INSTITUTE FOR POLYMERS AND COMPOSITES

# Outline



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# Outline

What is the main goal of the training section:

- Calculation of the forcing term
- Implementation of the forcing term in the solver
- Implementation of appropriate boundary conditions
- Calculation of error norms

“standard OpenFoam” and through `coded` functionality

- Mesh refinement study/ Code verification

Requirements:

- Some knowledge on Python programming
- Some knowledge on C++ programming (in the context of the OpenFOAM® framework)

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# Method of Manufactured Solutions

> ➢ **Code verification is an essential part of code development.**
>
> The verification of numerical codes consists in demonstrating that the code is correctly implemented, thus, for a progressively finer discretization the results will approach the mathematical solution.

- The OpenFOAM® framework has a vast collection of solvers for different continuum mechanics problems. However, due to the nature of the partial differential equations (PDE) being solved, the verification procedure is commonly made with an exact solution considering a simplified domain and/or simplified version of the original PDE.
  - This will hide possible problems in the code, due to not exercising every term in the PDE and/or limiting the shape complexity of the domain.

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**A more robust and general procedure for code verification is the method of manufactured solutions (MMS) where a solution (function) is predefined, and a forcing term is added to the PDE to drive its solution to the imposed function.**

# Method of Manufactured Solutions

$$Lu = S_T$$

Example

$$-\nabla \cdot \left( D_T \nabla T \right) = 0$$ → PDE

$$T = \cos\left(\alpha x\right) + \sin\left(\beta y\right)$$ → Manufactured solution

$$S_T = -\nabla \cdot \left( D_T \nabla \left[ \cos\left(\alpha x\right) + \sin\left(\beta y\right) \right] \right)$$

$$S_T = D_T \left( \alpha^2 \cos\left(\alpha x\right) + \beta^2 \sin\left(\beta y\right) \right)$$ → Calculation of source term

$$-\nabla \cdot \left( D_T \nabla T \right) = D_T \left( \alpha^2 \cos\left(\alpha x\right) + \beta^2 \sin\left(\beta y\right) \right)$$ → Final PDE

Where:

- $L$ is a differential operator,
- $u$ is the unkown,
- $S_T$ is a source term.

## Boundary conditions

Dirichlet:

$$T = g^D\left(x, y, z, t\right)$$

Neumann:

$$\frac{\partial T}{\partial \vec{n}_f} = \nabla T \cdot \vec{n}_f = g^N(x, y, z, t)$$

Robin:

$$\omega T + (1 - \omega) \frac{\partial T}{\partial \vec{n}_f} = g^R(x, y, z, t)$$

## Initial condition

$$T(x, y, z, t = 0) = T^0(x, y, z)$$

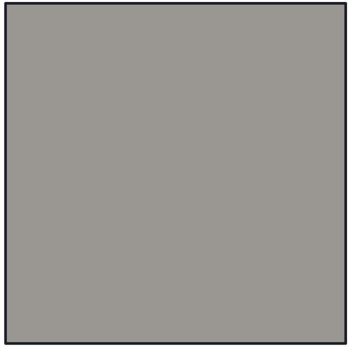
# Method of Manufactured Solutions

When we discretize the governing equations, we are subdividing the domain of the problem into finite volumes. Instead of solving the partial differential equation in a continuous domain, the equations are solved on a discrete space, which approximates the continuum solution.

"The approximate solution, which satisfies the discretized equations, is not the same as the exact solution which satisfies the mathematical continuum equations. The difference between the two is called **the discretization error**.

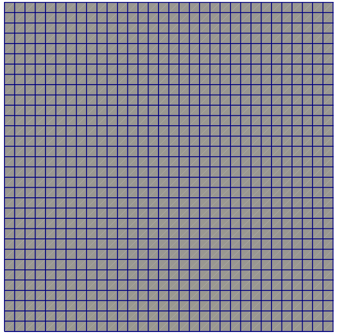
Discretization methods are named ***consistent*** if the error tends to zero as the representative cell size $h$ decreases to zero." [1]

The error decreasing rate is called the **convergence rate/ convergence order**.



Continuous domain

$$\int_V \nabla\cdot\left(\Gamma\nabla\phi\right) dV = \oint_S \Gamma\left(\vec{n}_f\cdot\nabla\phi\right) dS$$
$$= \sum_f \oint_{S_f} \Gamma\left(\vec{n}_f\cdot\nabla\phi\right) dS = \sum_f \Gamma_f \vec{S}_f\cdot\left(\nabla\phi\right)_f$$



Discretized domain

# Method of Manufactured Solutions

## Mesh refinement ratio

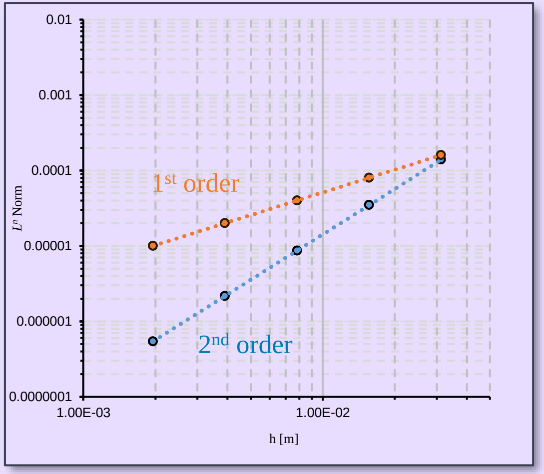
$$r = \frac{h_1}{h_2} \approx \left(\frac{N_1}{N_2}\right)^{\frac{1}{D}}$$

## Convergence order

$$p = \frac{\ln\left(\dfrac{L^{norm}_{coarse\ mesh}}{L^{norm}_{fine\ mesh}}\right)}{\ln(r)}$$

**Where:**

- $r$ is the refinement ratio
- $N_1$ is the number of cells in the fine mesh
- $N_2$ is the number of cells in the coarse mesh
- $D$ is the dimension of the problem (*1D, 2D or 3D*)




$$L^2 = \sqrt{\frac{1}{N}\sum_n \left(\phi_{FVM,n} - \phi_{MMS,n}\right)^2}$$

Or, more generally

$$L^2 = \sqrt{\frac{\sum_n \left(\phi_{FVM,n} - \phi_{MMS,n}\right)^2 V_n}{\sum_n V_n}}$$

**Other error norms:**

$$L^1 = \frac{\sum_n \left|\phi_{FVM,n} - \phi_{MMS,n}\right| V_n}{\sum_n V_n}$$

$$L^\infty = \max\left(\left|\phi_{FVM,n} - \phi_{MMS,n}\right|\right)$$

**Where:**

- $N$ is the number of cells in the mesh
- $\phi_{MMS,n}$ is the value of the manufactured solution at cell $n$
- $\phi_{FVM,n}$ is the value of the discrete solution at cell $n$
- $V_n$ is the volume of cell $n$

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# Method of Manufactured Solutions - `laplacianFoam`

`laplacianFoam` is a “basic” `OpenFOAM®` solver dealing with unsteady diffusion of a scalar quantity $T$.

Its governing equations is:

$$\frac{\partial T}{\partial t} - \nabla \cdot \left( D_T \nabla T \right) = S_T$$

**Where:**

$T$ is the scalar unknown quantity that evolves along time

$D_T$ is the diffusion coefficient

$S_T$ is a source term

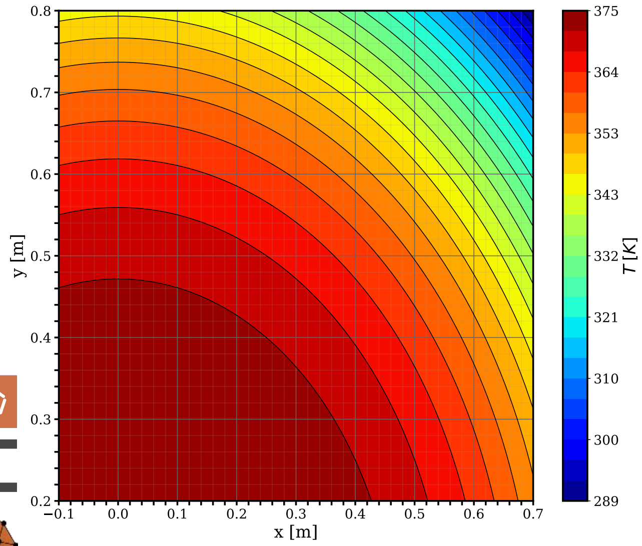
**Let us use the method of manufactured solutions with `laplacianFoam`**

# Method of Manufactured Solutions - `laplacianFoam`

Consider a 2$D$ **steady** case where the temperature solution is defined as:

**MMS**

$$T(x,y)=150\left[\cos\left(x^2+y^2\right)+1.5\right]$$




**Governing Equation**

$$\frac{\partial T}{\partial t}-\nabla\cdot\left(D_T\nabla T\right)=S_T$$

**Given that:**

$$\frac{\partial T}{\partial t}=0$$

$$D_T=1\times10^{-5}\quad\left[m^2s^{-1}\right]$$

All Dirichlet boundary conditions

Grid refinement study considering:

- M1: 32 x 32 x 1
- M2: 64 x 64 x 1
- M3: 128 x 128 x 1
- M4: 256 x 256 x 1
- M5: 512 x 512 x 1

- Compute the error norms
- Access the order of convergence

# Method of Manufactured Solutions - `scalarTransportFoam`

`scalarTransportFoam` is a “basic” `OpenFOAM®` solver dealing with the passive transport of a scalar quantity $T$.

Its governing equations is:

$$\frac{\partial T}{\partial t} + \nabla \cdot \left( \vec{v} T \right) - \nabla \cdot \left( D_T \nabla T \right) = S_T$$

**Where:**

$T$ is the scalar unknown quantity that evolves along time

$\vec{v}$ is the velocity

$D_T$ is the diffusion coefficient

$S_T$ is a source term

**Let us use the method of manufactured solutions with** `scalarTransportFoam`

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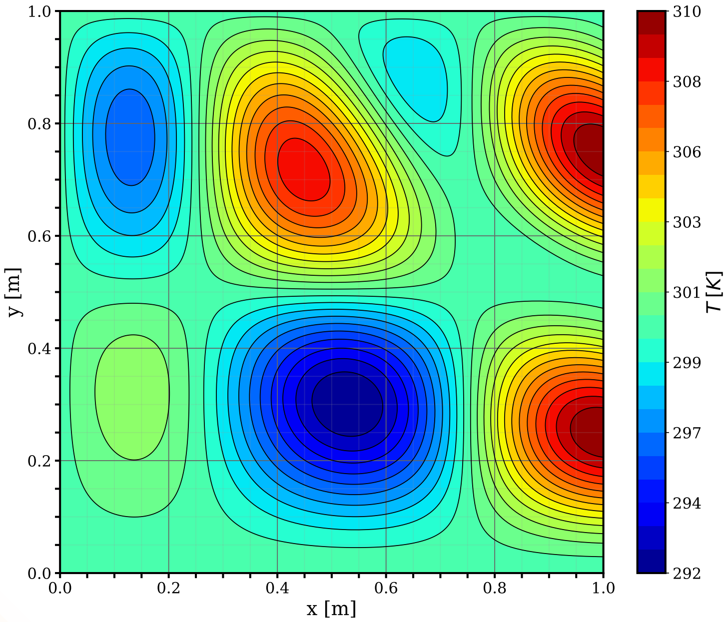
# Method of Manufactured Solutions - `scalarTransportFoam`

Consider a $2D$ **steady** case where the temperature solution is defined as:

**MMS**

$$T(x,y) = 300 + 10\sin(2\pi y)\sin(2\pi xy)\cos(2\pi x)$$




**Governing Equation**

$$\frac{\partial T}{\partial t} + \nabla\cdot(\vec{v}T) - \nabla\cdot(D_T \nabla T) = S_T$$

**Given that:**

$$\frac{\partial T}{\partial t} = 0$$

$$D_T = 1\times10^{-3} \qquad [m^2 s^{-1}]$$

$$\vec{v} = [0.1 \quad 0.1 \quad 0] \quad [m\, s^{-1}]$$

All Dirichlet boundary conditions

Grid refinement study considering:

- M1: 32 x 32 x 1
- M2: 64 x 64 x 1
- M3: 128 x 128 x 1
- M4: 256 x 256 x 1
- M5: 512 x 512 x 1

- Compute the error norms
- Access the order of convergence

# References

[1] - Kambiz Salari and Patrick Knupp, “Code Verification by the Method of Manufactured Solutions”, Sandia National Laboratories, 2000.

**Other relevant literature:**

[2] - P. J. Roache, “Code verification by the method of manufactured solutions,” J. Fluids Eng. Trans. ASME, vol. 124, no. 1, pp. 4–10, 2002, doi: 10.1115/1.1436090.

[3] - B. Blais and F. Bertrand, “On the use of the method of manufactured solutions for the verification of CFD codes for the volume-averaged Navier-Stokes equations,” Comput. Fluids, vol. 114, pp. 121–129, 2015, doi: 10.1016/j.compfluid.2015.03.002.

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[5] - C. Beisbart and N. J.Saam, Eds., “Computer Simulation Validation: Fundamental Concepts, Methodological Frameworks, and Philosophical Perspectives”, Chapter 12, pp.295-318, 2019.

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# Thank you for your attention