SAMOFAR

LPSC Grenoble

UNIVERSITÉ Grenoble Alpes

DEVELOPMENT AND IMPLEMENTATION OF AN ADAPTED TURBULENT MODEL IN OPENFOAM

APPLICATION TO LIQUID FUEL NUCLEAR REACTORS

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Outline

1. Introduction
   - The Molten Salt Fast Reactor (MSFR)
   - Challenges
2. The SWATH Experiments
   - Experimental design
   - Influence of Turbulence
3. GEATFOAM
   - GEATFOAM
   - Examples

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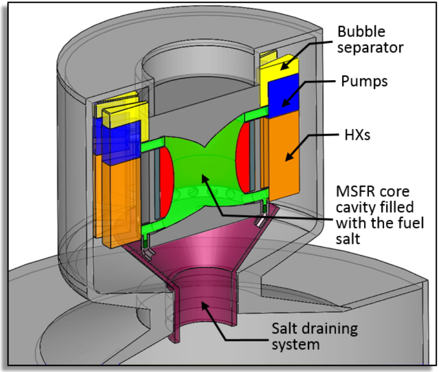
The Molten Salt Fast Reactor

Characteristics

- **Nuclear reactor**
- **Liquid fuel**: molten salt $LiF\text{-}ThF_4\text{-}^{233}UF_4$
- **High mean operation temperature** $= 725^\circ C$
- **High temperature rise over the core** $\approx 100^\circ C$
- **High melting point for the molten salt** $= 585^\circ C$
- **3D flow** $Re \approx 10^5$

The core of the nuclear MSFR



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Challenges

Characteristic	Challenge
Liquid fuel	Fields coupling
High operation temperature	Radiative heat tranfer
High temperature rise over the core	Errors introduced by the Boussinesq approximation
High melting point for the molten salt	Phase change: Solidification
3D flow	Large impact of turbulence on the flow characteristics

Table: Challenges introduced for a high temperature coolant

Figure: Fields coupling for the MSFR

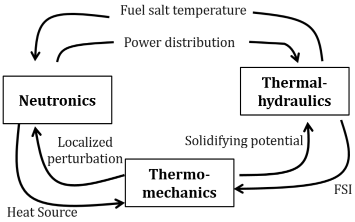
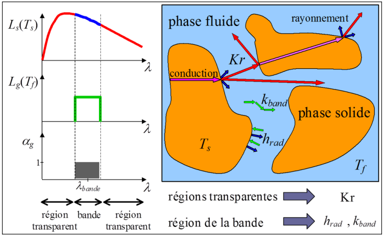


Figure: Radiative transfer model



Ongoing work on my PhD thesis . . .

- **Understand the thermal hydraulics behaviour** of a high temperature molten salt coolant and **development of specific models** for determining its field equations.
- These models have to be **validated by experiments**. The complexity of the flow phenomena requires a careful design of the experiments for a step by step validation the models.
- The **SWATH (Salt at WAlls: Thermal excHanges) project** was started at LPSC for developing these experiments. The SWATH project is a part of the European collaboration project SAMOFAR that aims to demonstrate the innovative safety approaches of the Molten Salt Fast Reactor.
- The **thermal-hydraulics models** have been **coupled** to **neutronic codes** and will be coupled to subsequent **thermal mechanics models** for performing full scale simulations of the MSFR.

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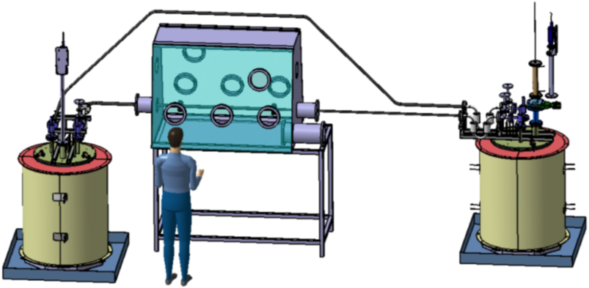
The SWATH Project

- **Principle of operation**: The flow is established by the **over pressure** of one tank with respect to the other.
- A **test section is included in the circuit**, enclosed in a glove box.
- Due to the high corrosion properties of the fluoride salt and the high temperature of operation only Stainless Steels are used as materials.
- The **experiment instrumentation** and the **measurements** are difficult.

Figure: SWATH model



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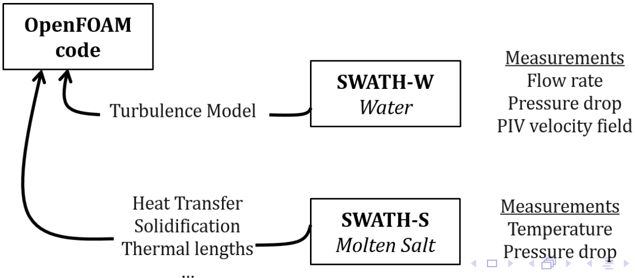
Hydraulic modeling is a key point in the SWATH experiments

- For the geometries to be used in the test sections the **RANS models** introduce **errors of** $\pm 5 - 10\%$ in the calculations.
- For **LES** and **hybrid methods** the implicit dissipation of the scheme choose as well as the extent of the buffer layer usually requires **a good a-priori knowledge of the searched solution in order to produce accurate results** and **they are too computationally demanding** for the amount of calculations needed in the design of the experiences.
- Since the particular physical phenomena of the molten salt (solidification, radiative heat transfer, boundary layer developement, etc.) accounts for uncertainties of $\sim 10\%$ **an error of** $\pm 5 - 10\%$ **on the turbulence models is not acceptable.**
- Furthermore, **the molten salt flow fields can't be measured directly**.

Dimensionally Similar Test Sections

- **Two similar facilities** are designed for operating with water (SWATH-W) and with molten salt (SWATH-S) and each test section is constructed **with the same dimensions** for SWATH-W (Plexiglas) ans SWATH-S (Stainles Steel).
- The turbulent models for the test section geometries are **validated** by the measurements in SWATH-W and by dimensional similarity, maintaining the *Re* number, the models can be **extended** to SWATH-S.

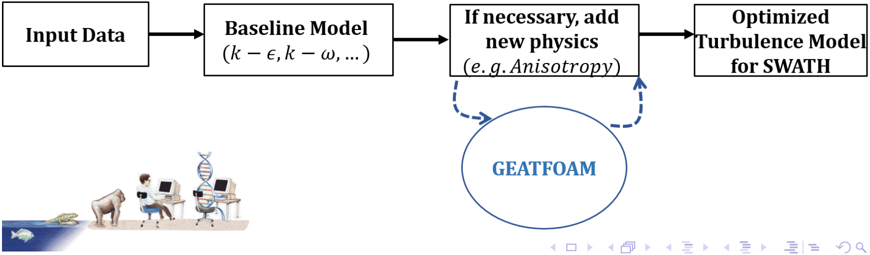
Figure: Strategy for validating the turbulent models for SWATH-S



Turbulence Model Optimization Tool: GEATFOAM

- Rather than a specific model, **a tool is needed** to **adapt existing RANS turbulence models** to the test sections in SWATH.
- A **Genetic Evolutionary Algorithm** for **Turbulence** models creation was developed and coupled to **OpenFOAM** (GEATFOAM).
- The Genetic Evolutionary Programing (GEP) technique was chosen for its simplicity and the possibility to implement symbolic regression.

Figure: GEATFOAM turbulent model development process



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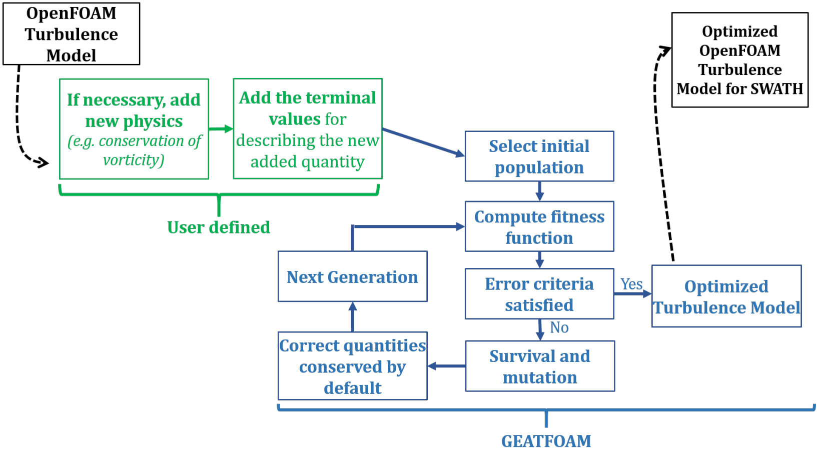
Evolutionary Structure of GEATFOAM

Figure: Internal structure of the turbulence model optimization process



Implementation as a turbulence models in OpenFOAM

Incompressible Turbulence Models Libraries

"libIncompressibleRASModels.so"
"libIncompressibleLESModels.so"

turbulenceModel.H

- Define headers of the parameters: tmp<volScalarField>
- Define in-line functions and constructors: tmp<fvScalarMatrix>

turbulenceModel.C

- Calculate the parameters: tmp<volScalarField>
- Solve the turbulent model equations: tmp<fvScalarMatrix>

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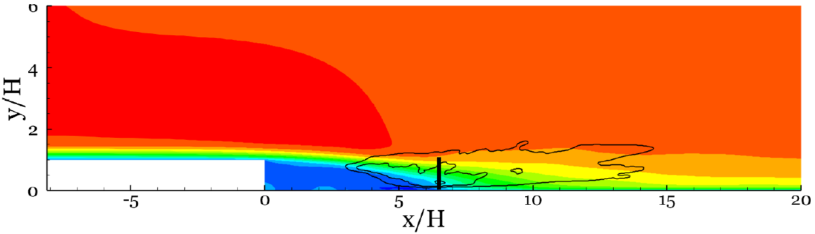
Example 1: Backward Facing Step as ERCOFTAC

Figure: DNS simulation of a Backward Facing Step as ERCOFTAC to be used as training data. Filled by mean stream-wise velocity U, lineas are the ratio v^{rms}/u^{rms} at contour values 0.4, 0.6 and 0.8



- **Conventional RANS models** $(k-\epsilon, k-\omega, \ldots)$ **produce large errors** in the velocity fields down the step and the boundary layer reattachment point.
- The produced **turbulent field in the inferior region is not isotropic** before the reattachment of the boundary layer.
- RANS models assume isotropic turbulence.

Proposed modified model with anisotropy

Modified Baseline k-ω model as (Menter, 1994)

$$\partial_t k + U_j \partial_{xj} k = P_k - \epsilon + \partial_{xj}[(\nu + \sigma_k \nu_t)\partial_{xj} k]$$

$$\partial_t \omega + U_j \partial_{xj} \omega = \gamma\omega/kP_k - \beta\omega^2 + \partial_{xj}[(\nu + \sigma_\omega \nu_t)\partial_{xj}\omega] + \sigma_d CD^+_{k\omega}$$

$$\overline{u'_i u'_j} = 2/3\delta_{ij} k - 2\nu_t S_{ij} + a^x_{ij}$$

a^x_{ij} is taken as 0 for the SST model

see (Hellsten, 2005) for more details

Terminal values and fitness function

Anisotropy models

$$a_{ij}^{x} = a_{ij}^{x}(k, \epsilon, S_{ij}, \Omega_{ij}) \text{ (Pope,1975)}$$

S_{ij} is the mean share rate tensor and Ω_{ij} is the rotational of the mean velocity

The chosen terminal functions are 4 tensors and 2 invariants:

$$T^1 = S_{ij},\ T^2 = S_{ik}\Omega_{kj} - \Omega_{ik}S_{kj}$$

$$T^3 = S_{ik}S_{kj} - 1/3\delta_{ij}S_{mn}S_{nm},\ T^4 = \Omega_{ik}\Omega_{kj} - 1/3\delta_{ij}\Omega_{mn}\Omega_{nm}$$

$$I^1 = S_{mn}S_{nm},\ I^2 = \Omega_{mn}\Omega_{nm}$$

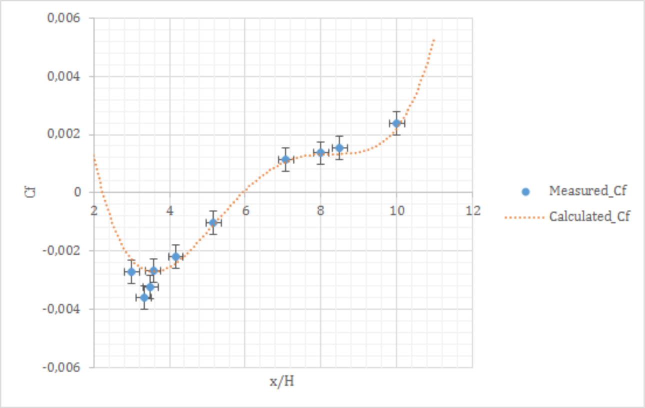
Fitness function

$$f(P_i^j) = \frac{a_{mn}^{DNS}\, a_{mn}^{GEP}}{(a_{pp}^{DNS})^{1/2}(a_{qq}^{GEP})^{1/2}}$$

Where a_{mn}^{DNS} is the raw DNS anisotropy and a_{mn}^{GEP} is the current anisotropy of the genetic evolutionary program.

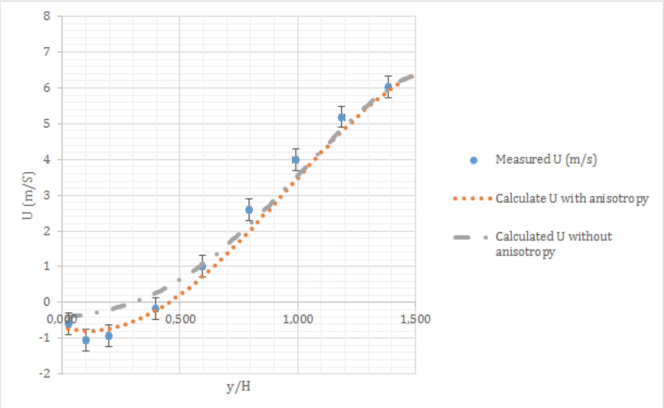
Skin Friction Coefficient

Figure: Comparison of the optimized model against experimental measurements [5] for the friction coefficient in the inferior wall. The global difference is calculated in 1.6%



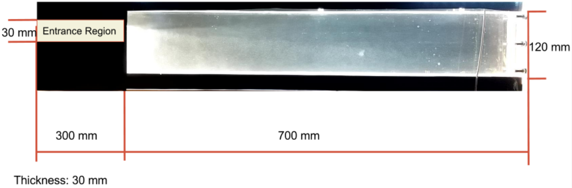
Streamwise velocity and Reynolds shear stresses

Figure: Comparison the streamwise velocity for the models with and without anisotropy on the line $x/H = 4.0$ model against experimental measurements [5]. The gobal difference is 1.2% for the model with anisotropy considerations and 4.6% for the one without.

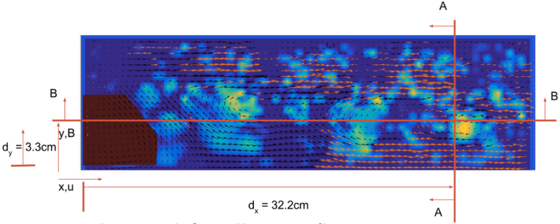


Example 2: Backward Facing Step with Big Expansion

Experiment built at LPSC on the forced convection loop experience.



Preliminary Particle Image Velocimetry measures taken of the experiment.



The experiment was designed for allowing flow streamwise inversion in the inferior part.

Example 2: Backward Facing Step with Big Expansion

Baseline Extended Standard k-ϵ model as (Chen, 1987)

$$\partial_t k + \partial_{x_i} k u_i = \partial_{x_j}[\nu + \nu_t/\sigma_k]\partial_{x_j} k + P_k + P_b - \epsilon$$
$$\partial_t \epsilon + \partial_{x_i} u_i \epsilon = \partial_{x_j}[\nu + \nu_t/\sigma_\epsilon]\partial_{x_j}\epsilon + C_{1\epsilon}\epsilon/k(P_k + P_b C_{3\epsilon}) - C_{2\epsilon}\epsilon^2/k$$

The general closure taking into account up to third order temrs is:

$$\rho\overline{u_i' u_j'} = -\mu_t S_{ij} + \frac{2}{3}k\delta_{ij} +$$
$$\sum_{m=1}^{2}\sum_{n=1}^{2} C_{2mn}\mu_t \frac{k}{\epsilon}[(\vec{H}_{ik}\vec{H}_{kj})_{mn} - (\vec{H}_{lk}\vec{H}_{lk})_{mn}\delta_{ij}\delta_{mn}] +$$
$$+ \sum_{m=1}^{3}\sum_{n=1}^{3} C_{3mn}\mu_t \frac{k^2}{\epsilon^2}(\vec{H}_{ij}\vec{H}_{kl}\vec{H}_{op})_{mn}$$

Where $\vec{H}_{ij} = [S_{ij}\,\Omega_{ij}]$, S_{ij} is the mean share rate, Ω_{ij} is the rotational of the mean velocity and $\vec{H}\vec{H}$ accounts for the dyadic expansion of vector H

see (Bardina et. al., 1997) for more details

Example 2: Backward Facing Step with Big Expansion

Cubic closure term modelling

9 tensors are proposed as initial terminal population as well as 6 independent invariants of this one. Respectively they read in $\mathbb{R}$

- Tensors: $H_{ij} = (H_{lk} HkmHij)$
- Invariants: $H_{ij} = I((H_{lk} HkmHmn))$

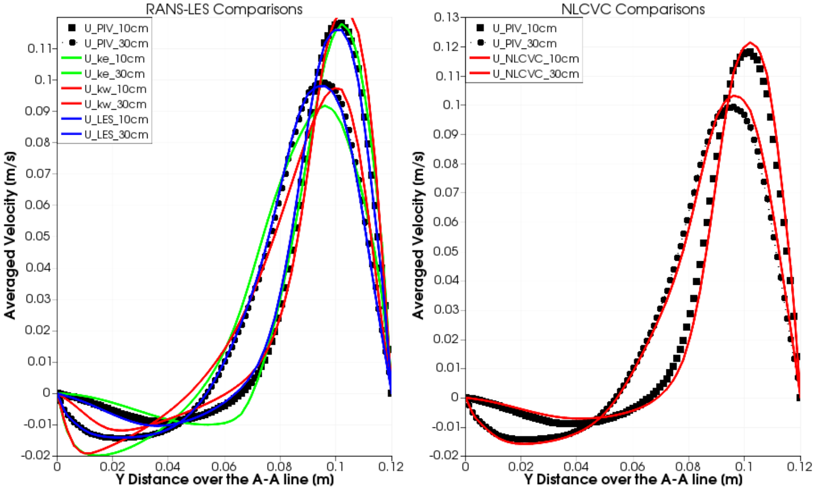
Fitness function

$$f(P_i) = var(P_1, \ldots, P_n)$$

Where P_i is an individual population and n is the number of individuals in the population defined by the selection criteria and the amount of information contained in the plasmid for the present case.

Results: streamwise average velocity

Preliminary PIV measurements



Comparison of the GEP model (right) against high accuracy LES simulations and standard RANS models (left). The global error of the Non Linear Cubic Vorticity Conservative Model (NLCVC) is 1.2%

Summary

- The SWATH project at LPSC will help us understand the physical behaviour of a molten salt flow and to experimentally validate numerical models for their description.
- The GEATFOAM tool is an optimization tool for turbulence models capable of improving the turbulent model for a defined experiment.

- Outlook
  - Further work needs to be done in the development and validation of the GEATFOAM tool.
  - A better definition of the optimization space can be done for improving the convergence speed of GEATFOAM.

Thanks for your attention..!

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For Further Reading I

W.H. Steeb.
The nonlinear workbook: chaos, fractals, cellular automata, neural networks, genetic algorithms, gene expression programming, support vector machine, wavelets, hidden Markov models, fuzzy logic with C++, Java and SymbolicC++ programs..
World scientific, 2011.

B. Fabritius.
Application of Genetic Algorithms to Problems in Computational Fluid Dynamics
PhD Thesis, 2014.

For Further Reading II

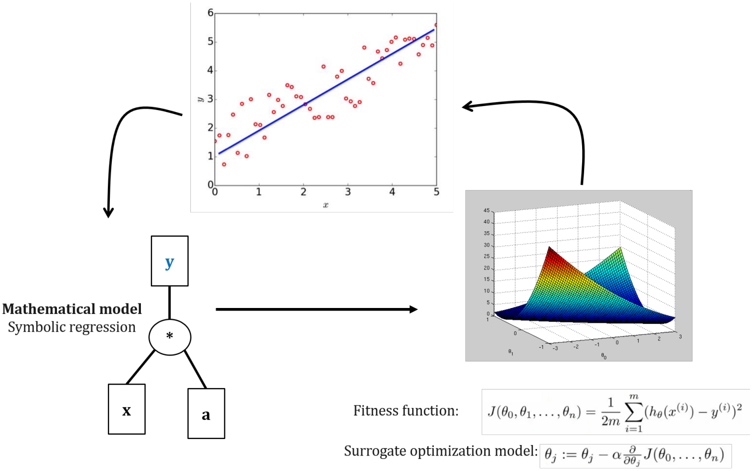
J. Weatheritt.
The development of data driven approaches to further turbulence closures
PhD Thesis, 2015.

S. Yarlanki. et. al.
Estimation of turbulence closure coefficients for data centers using machine learning algorithms
ITherm, $13^t h$ IEEE Intersociety Conference, 2012.

Jovic, S., Driver, D. M.
Backward-facing step measurements at low Reynolds number, $Re_h = 5000$.
NASA, 1994.

Principles of evolutionary optimization used

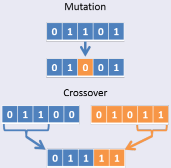
Figure: Mathematical model and fitting of a scalar regression problem.



Theoretical Background

Mutation Mechanisms

- Cross-over
- A small amount of self mutation



Space of Optimization

- **Scalar Regression:** $\phi : \mathbb{R}x \ldots x\mathbb{R} \to \mathbb{R}$
- **Optimization Space:** $T : V^1 \otimes V^2 \otimes V^3 \to W^1 \otimes W^2 \otimes W^3$, where $V^i \in \mathbb{R}^3$, $W^i \in \mathbb{R}^3$
- On this space the set of **functions for optimization** is defined as: $F = \{+ : +, - : -, * : F(A_{ij}, B_{ij}) \to A_{ik}B_{kj}, T : T(A_{ij}) \to A_{ij}\}$ and the **terminal set**: $T = \{A : A_{ij}, B : B_{ij}, I : \delta_{ij}, ? : RNC_{ij}\}$