Salome_CFD user meeting 2019 Salome_CFD Highlights

Salome_CFD development team¹

7th May 2019





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Outlines

1 Introduction

2 Main news in version V6.0 and upcoming perspectives

- Pre- and postprocessing
 - User settings and GUI
- Physical modelling
- Numerics
 - Interoperability
- 3 Conclusion and discussion











Salome_CFD Highlights [4/43]







Salome_CFD Highlights [4/43]





Advanced scripting capabilities











Single-phase solver *Code_Saturne* Multi-phase solver NEPTUNE_CFD



Salome_CFD Highlights [4/43]







Visualisation / Remote visualisation for Big Data







Visualisation / Remote visualisation for Big Data In-situ and live visualization











UQ studies Design





Multiphase solver developed in the NEPTUNE project (EDF, Framatome, CEA, IRSN): NEPTUNE_CFD

- → Multi-fluid, Eulerian model (one-pressure, "Ishii" class of models)
- → Dedicated sets of physical models to tackle a wide range of two-phase flows with different topologies (stratified, dispersed, etc.)
- → Inherits many capabilities from Code_Saturne: HPC, pre/post-processing, GUI, linear algebra, data structures...
- → Not open-source

Some target nuclear applications:

- → Departure from Nuclear Boiling (DNB)
- → Two-phase Pressurized Thermal Shock (PTS)
- → Containment flows (with aspersion and condensation)
- \rightarrow Gas transport in pipes
- → Downcomer during a LOCA
- → Spent-fuel pool in case of accident
- → In-vessel corium retention







Thermal diffusion in solids and radiative transfer solver: SYRTHES

Thermal load of 1000 bolts in 900 PWR internals

1h30 on 2048 BG cores - 1 billion tet mesh



Solid coupled to fluid (Code_Saturne)





Multiphysics solvers gathered in Code_Saturne





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Salome_CFD Highlights [10/43]











see user source file cs_user_mesh-modify.c.

edF

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Preprocessing: automatic insertion of wall-layer cells Fix features in sharp angles

A solution is to test for negative volumes while deforming the mesh, and locally limit the extrusion on adjacent boundaries (removing

one extrusion layer at vertices of those cells). This is done iteratively until no negative volume cells are produced.



before



Also add optional cell volume ratio limiter to reduce the extrusion near cells that would be excessively flattened or entangled.





CALIFS

Preprocessing: Add mesh refinement engine

for any polyhedral, load balancing currently handled through complete repartitioning, in collaboration with STFC



see function cs_user_mesh-modify.c.



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Add restart function to allow mapping restarts from computation using a different mesh







Code_Saturne & NEPTUNE_CFD now in the same GUI

Switch between Code_Saturne and NEPTUNE_CFD solvers

It is now possible to easily switch between the *Code_Saturne* solver (Standard Eulerian single-phase) and NEPTUNE_CFD solver (Eulerian Multiphase) using the GUI:







Improving the global workflow of a study

- → Manage User functions within the GUI!
- \rightarrow View log files of a run

Calculation environment Calculation environment Constant Const	Flow Models Standard Eulerian single phase Atmospheric Electric ars Groundwater Reactive flows (combustion) Eulerian molitiphase NMPPINME (CFD)	Incompressible v
n Outpute samg	Additional Features Eulerian Lagrangian model Turbomachinery model Deformable mesh (ALE method) Fans (source-term model)	off v





Improving the global workflow of a study

- → Manage User functions within the GUI!
- \rightarrow View log files of a run

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Improving the global workflow of a study

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- \rightarrow View log files of a run

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Improving the global workflow of a study

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Improving the global workflow of a study

- $\rightarrow\,$ Manage User functions within the GUI!
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Coupled NEPTUNE_CFD/CATHARE2 cases

Creating a coupled NEPTUNE_CFD/CATHARE2 case

neptune_cfd create -c NEPTUNE –cathare CATHARE

Case parameters handling

Coupling can be handled using GUI and coupling_parameters.py file

Activate coupling ~

fluid phases to couple	fluid phases to couple 💿 Main continuous phase 💿 All phases					
NEPTUNE_CFD INSTANCE	NEPTUNE					
CATHARE2 INSTANCE	CATHARE					
Cathare data file	catharejdo	i.dat				
Coupling name	NEPCAT_C	PL				
Cathare initialize time	0.0					
Coupling time to simulate	0.0					
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TUBE2 1	2	Pipe_exit		x > 0.9		
			Add	Delete		
	_					





Turbulence heat flux modelling

→ Elliptic Blending Differential Flux Models for scalars (EBDFM ityturt = 31)
→ Give very good results, especially wall bounded and flow with buoyancy

Similarly to EB-RSM the scrambling/dissipation terms $\Phi_{ij}^* / \varepsilon_{ij}$ are computed via the parameter α_{θ} ($\alpha_{\theta} \in [0, 1]$). It is used to **blend the fully turbulent and the viscous regions** (DFM $\iff \alpha_{\theta} = 1$)

$$(\Phi_{i\theta}^* - \epsilon_{i\theta}) = (1 - \alpha_{\theta})(\Phi_{i\theta}^w - \epsilon_{i\theta}^w) + \alpha_{\theta}(\Phi_{i\theta}^h - \epsilon_{i\theta}^h)$$

→ Elliptic Blending version of GGDH and AFM (EBGGDH ityturt = 11 and EBAFM ityturt = 21)



 \rightarrow 1D channel flow (Dirichlet on T)

Major **improvement** for the prediction of **fluctuations** and **temperature variance** compared to **standard models**





Changes and new turbulence models

Changes in the k- ω -SST model

- → In the near wall region (see Menter): Dirichlet on $\omega_f = 10 \times \frac{6\nu}{\beta d}$, with *d* the cell center to cell face distance.
- → Now, to be coherent with other models and Menter: $\omega_f = \frac{5u_k^2}{\sqrt{C_\mu}\kappa\nu\gamma^+}$ back to the previous BC with ikycln = 0.

 \rightarrow Can be activated by setting iturb = 23







Velocity Mag 3.7e-03 0.5 1 1.4e+



for the Reynolds stresses

going to order $2 \rightarrow$ guadratic models

New quadratic $k-\varepsilon$ model from Baglietto et al. Theory of invariants \rightarrow generalized the idea of constitutive relation

It becomes $\underline{\mathbf{R}} = \mathbf{f}(\underline{\mathbf{S}}, \underline{\Omega})$ where $\underline{\mathbf{R}}$ is the Reynolds stress tensor. When

Reproduction of secondary flows due to anisotropy *E.g.* secondary flows in the square duct channel

Salome_CFD Highlights [20/43]

All y^+ treatment

Wall functions for the EB-RSM are available with *iwallf* = 7 and activated as default.

- Simplified version of J.F Wald PhD (2016)
- Ensure convergence towards standard EB-RSM when mesh is refined
- Degenerate in a SSG-like model on high Reynolds meshes
- \rightarrow New continuous wall function on the velocity and the velocity gradient
- \rightarrow Similarly to $k \omega$ SST model, in high Reynolds zones, we use $\varepsilon_f = \varepsilon_{I'} + d \left. \frac{d\varepsilon}{dy} \right|_{d/2}$ to impose appropriate BCs on ε . This is blended to the wall behaviour through a blending function $f_{\varepsilon}(y^{+})$.

 \rightarrow Homogeneous Neumann BC on Reynolds stresses, except $R_{12} = C_{\alpha} \sqrt{R_{11}R_{22}}$, $C_{\alpha} = 0.47$



All y^+ treatment

New iwallf = 7 can be activated with the $k - \omega$ SST.

- \rightarrow Default wall functions (iwallf = 3), can also be used as an all y⁺ treatment
- → Be careful to avoid buffer layer $5 < y^+ < 20$

A low Reynolds $k - \varepsilon$ model (Launder and Sharma, 1974) is available (iturb = 22).

- \rightarrow Default wall functions (iwallf = 3), can be used as an all y⁺ treatment
- → New iwallf = 7 can be activated



Delayed Detached Eddy Simulation

- \rightarrow Hybrid RANS/LES model (Spalart 2006) for *k*- ω -SST model
- → Mesh requirements between U-RANS and LES



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Mean skin friction coefficient



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The turbulent length scale

$$\tilde{L} = f_d L_{LES} + (1 - f_d) L_{RANS}$$

is blended with $f_d \in [0, 1]$

- → Improvement in velocity predictions
- → Better level of turbulent kinetic energy
- → Reattachement point in agreement with LES



Solidification modelling within *Code_Saturne* See dedicated presentation by C. Demay (EDF R&D/PRISME)

Objectives: study of carbon segregations during ingots casting Modeling: fluid / solid mixing model with motionless solid phase

$$\begin{pmatrix} \operatorname{div} \left(\rho \underline{u}\right) = 0 \\ \frac{\partial \rho \underline{u}}{\partial t} + \underline{\operatorname{div}} \left(\underline{u} \otimes \rho \underline{u}\right) = -\underline{\nabla}P + \underline{\operatorname{div}} \mu_{l} \underline{\nabla}\underline{u} \\ -\frac{\mu_{l}}{K} \underline{u} + \rho^{b} (T, C_{l}) \underline{g} \\ C_{p} \left(\frac{\partial \rho T}{\partial t} + \operatorname{div} (T\rho \underline{u})\right) = \operatorname{div} \lambda \underline{\nabla}T - \frac{\partial \rho g_{l} L}{\partial t} \\ \frac{\partial \rho C^{\alpha}}{\partial t} + \operatorname{div} \left(C^{\alpha} \rho \left(1 + \eta^{\alpha}\right) \underline{u}\right) = \operatorname{div} K \underline{\nabla}C^{\alpha}$$

Microsegregation model, binary phase diagram ($g_I(T, C)$) and Boussinesq Hyp. Work in progress combining several features:

- → PISO-like sub iterations (10)
- → Buoyancy: C and T are solved in the sub-iterations (is_buoyant field key word)
- → Uses "improved hydrostatic treatment"
- → Uses "porous" modelling (to cancel mass fluxes in the solid zones)
- → Conjugated heat transfer with internal coupling

Work done within M.-A. Rasendra internship and continued with EDF China and a thesis.





Solidification modelling within Code_Saturne

Validation testcase preview (versus SOLID)...







Solidification modelling within *Code_Saturne* Validation testcase preview (versus SOLID)...

Liquid fraction g_l

Time: 204.010000







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Solidification modelling within Code_Saturne

Validation testcase preview (versus SOLID)...



Add a compressible 2-phase homogeneous model

Work of O. Hurisse (EDF R&D/MFEE)

- → fractional step method sharing mass, momentum, energy balance steps with single phase compressible algorithm
- → convection and source terms (relaxation towards equilibrium) step for each fraction (volume, mass, energy) follow
- \rightarrow thermodynamic of the mixture is generic
- → each phase thermodynamics follows a stiffened gas EOS (parameters are at hand for the user)
- → relaxation time scale of return to equilibrium also at hand for the user
- → the model can be activated by setting to 2 the physical model parameter cs_glob_physical_model[CS_COMPRESSIBLE]





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Salome_CFD Highlights [26/43]

Two major modelling advances in NEPTUNE_CFD

Towards the modelling of two-phase flow regime transition

Generalized Large Interface Method (GLIM) available and validated on a collection of adiabatic two-phase flows with different regimes (see technical presentation)



Modelling the motion of solids in two-phase flows

An innovative method to simulate the motion of solid structures (user- or flow-imposed) is now available (see dedicated presentation + demo)





Changes in default option of linear solvers

- → Default solver for convection-diffusion changed to symmetric Gauss-Seidel ⇒ **Performance gain** slightly less than 2 expected
- → On BUNDLE benchmark case (12M cell variant), Pressure solution is unchanged at 202 seconds, velocity solution goes from 298 to 95 seconds, k from 115 to 43, epsilon from 31 to 12, total elapsed time from 893 to 606 seconds.



- → For internal coupling, Jacobi or Gauss-Seidel is not well adapted to resolution of systems with purely diffusive zones
 - → BiCGStab or BiCGStab2 recommended in these zones
 - → since occasional divergence of these solvers is observed (1 every 500 to 1500 time iterations), temporary fallback to slower, but more robust GMRES is applied automatically.







CDO roadmap (See Groundwater flow pres. by J. Bonelle & R. Lamouroux)



CDO News

- \mapsto **Stokes** for Face-based schemes
 - Towards (Navier–)Stokes
 - Fully coupled (Velocity-Pressure) algorithm
 - Steady-state algorithm available
- → Vector-valued Laplacian in Vertex-based schemes
 - ALE module See dedicated presentation by J. Harris (ENPC)
- → Adding more general boundary conditions
 - Robin and sliding boundary conditions

→ Volumetric interpolation

• Enforcement of values inside the domain







Salome_CFD Highlights [31/43]

Porous modelling

Work done in C. Colas PhD - see his poster for more on the integral formulation

- \rightarrow Model a fluid section jump in an incompressible flow.
- → Tools: integral formulation cs_glob_porous_model = 3 with discontinuous porosity.
- → Situation before: uncorrect result due to linear interpolation of cell values to compute interface values (valid for C^1 fields).



Porous modelling Work done in C. Colas PhD - see his poster for more on the integral formulation

- → Solution: modified interpolation for interface values (field not differentiable) using a local steady balance on the dual sub-cells.
- \rightarrow Situation after: the piecewise constant velocity and pressure fields are recovered with the solver precision.



N.B. Rhie & Chow filter should be used and adapted when solving the pressure to avoid spatial oscillations.



Salome_CFD Highlights [33/43]



2nd order time scheme for variable density flow

- → Major changes in time stepping to ensure 2^{nd} order in time for variable density flow if 2^{nd} order time scheme is enabled. Scheme is similar to (C. Pierce, 2000).
 - Buoyant scalars and density update can be included in velocity-pressure loop. To enable it, use is_buoyant field key word.
 - □ The momentum equation is staggered in time, i.e. when 2^{nd} order is enabled, velocity is solved from time $n \frac{1}{2}$ to $n + \frac{1}{2}$.

Work done in collaboration with C. Flageul.



OECD Cold Leg Mixing CFD-UQ benchmark - R. Camy (EDF/DT).





Coupled solver for DRSM turbulence models (default)

 \rightarrow Goal: increase linear solver robustness, and ensure realisability of <u>R</u>.

Comparison between segregated and coupled versions



→ New time scheme allowed by the coupled solver in which more terms are made implicit.

Example: 100 iterations for each case from same initial state:

→ Faster convergence for the coupled version.





Coupled solver for DRSM turbulence models (default)

Improvement of the linear solver efficiency: **no clipping** at all for any of the components (dashed lines).



Number of clipped cells for each component of $\underline{\underline{R}}$. Total number of cells \approx 110 000.





Coupled solver for DRSM turbulence models (default)

Improvement of the linear solver efficiency: a better convergence of the linear solver







OpenTURNS- *Code_Saturne* workflow

1st version of full integration into Salome_CFD workbench

workflow example: compute $C_d = \frac{\Delta P}{\Delta r}$ on an orifice plate model.



			Press	ure			
-2.2e+00	-1.5	-1	-0.5	0	0.5	1	1.6e + 00



- 1 define input (Re) and output (ΔP) inside Code_Saturne's GUI
- 2 switch to OpenTURNS mode available in Code Saturne's GUI in Salome CFD
- define computational resources 3 (desktop, distant HPC cluster) for a unitary run
- switch to OpenTURNS module and for example, define a DOE, here a set of Re values
- run all evaluations
- postprocess results inside 6 OpenTURNS, here C_d .



MEDCoupling support

MEDCoupling:

A library which is co-developed by EDF and CEA within the SALOME project. It is centered around mesh and fields manipulation, including interpolation.

Offers powerful functionnalities such as 3D/3D, 2D/2D or 3D/1D interpolation tools.

What is implemented:

- \rightarrow Sequential and Parallel remapping
- \rightarrow Parallel (MPI-based) code coupling





MEDCoupling support Example 1: 2D fields

Imposing a temperature field at an inlet





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Salome_CFD Highlights [40/43]



MEDCoupling support

Example 2: 3D fields

Time and space dependent porosity field



- → Configuration: a rotor in a fluid domain
- → On the fly computation of the fluid volume during the simulation.



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Get sources or binaries fitting your needs!

Git repository

- → Internal repository on PAM GitLab forge: https://gitlab.pleiade.edf.fr/salome_cfd and subprojects.
- → development tab on code-saturne.org now links to https://github.com/code-saturne/code_saturne public git mirror.
 - Bug reports and feature requests on matching issues section.
 - for confidential data or issues, use of the PAM GitLab issue tracker or saturne-support e-mail is possible.
- \rightarrow GitHub also provides a Wiki (to be populated).

Get Salome_CFD binaries

→ on *Code_Saturne* website https://www.code-saturne.org/cms/salome-cfd





Salome_CFD Highlights [42/43]



Conclusion messages

Code_Saturne is NOT a black-box! Ask what you want! Merci pour toutes ces années d'utilisation !

internal issue tracker (EDF users) https://gitlab.pleiade.edf.fr/ salome_cfd/code_saturne/issues

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external issue tracker (public) https://github.com/code-saturne/ code_saturne/issues

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