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> RUSSIAN ACADEMY OF SCIENCES Nuclear Safety Institute (IBRAE)

High Performance Computing for CFD problems and uncertainties quantification

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Workshop on Advanced simulation in support to GIF reactor design studies – Contribution of HPC and UQ"

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CONV3D code for numerical solving of Navier-Stokes equations

The time-dependent incompressible Navier-Stokes equations in the primitive variables for incompressible fluid together with energy equation:

(1.1)
$$\begin{cases} \frac{d\rho\vec{v}}{dt} = -\operatorname{grad} P + \operatorname{div} v \operatorname{grad} \vec{v} + \rho g & (1.2) \quad \frac{\partial(\rho h)}{\partial t} + \operatorname{div}(\rho v h) = \operatorname{div}(k \operatorname{grad} T) \\ \operatorname{div} \vec{v} = 0 & h = \int_{0}^{T} c(\xi) d\xi \end{cases}$$

3D CFD CONV code based on finite-volume methods and fully staggered grids.

For convection the nonlinear monotonic scheme is developed.

The Richardson iterative method with FFT as preconditioner is applied for solving of pressure equation.

The CONV code is fully parallelized and highly effective at the HPC "Chebyshev", "Lomonosov" .

(1.3)
$$\rho \frac{\mathbf{v}^{n+1/2} - \mathbf{v}^n}{\tau} + (C(v) - \operatorname{div} v \operatorname{grad}) \mathbf{v}^{n+1/2} + \operatorname{grad} p^n - \operatorname{CSF}^n = 0,$$

(1.4)
$$\operatorname{div}_h \left(\frac{1}{\rho} \operatorname{grad}_h \delta p \right) = \frac{1}{\tau} \operatorname{div}_h \mathbf{v}^{n+1/2}, \qquad \mathbf{v}^{n+1} = \mathbf{v}^{n+1/2} - \frac{\tau}{\rho} \operatorname{grad}_h \delta p .$$

Turbulence modeling

Different turbulence models are used

- Algebraic Models (Algebraic models work well for attached boundary layers under mild pressure gradients, but are not very useful when the boundary layer separates.)
 - Cebeci-Smith
 - Baldwin-Lomax (improves on the correlations of the C-S model and does not require evaluation of the boundary layer thickness. It is the most popular algebraic model.)
- One-Equation Models (1 pde)
 - Spalart-Allmaras (S-A) (can be used when the boundary layer separates and has been shown to be a good, general-purpose model; at least robust to be used for a variety of applications.)
- Two-Equation Models (2 pdes)
 - k-epsilon and its different modifications
- Models mostly assume fully turbulent flow rather than accurately model transition from laminar to turbulence flow.

CONV-3D scalability

Example: ERCOFTAC test using SMITH-solver (HPC Mira BlueGene/Q(ANL))



Validation : T-junction thermal mixing flow

Comparison of CONV3D numerical predictions to results experimental and computational results of Mahaffy (2010).

A test's singularity is that the hot fluid flows from a vertical pipe is poured into a horizontal pipe with a cold flux.

Computational geometry



CONV3D predictions are obtained at grid with 12 million nodes and marked by a dashed line (12M). CONV3D predictions are obtained at grid with 40 million nodes and marked by a solid line (40M).

Mahaffy predictions (2010) were obtained at grid with 7 million nodes and marked by stars (7M).

Experimental data are marked by circles.

John Mahaffy and Brian Smith, Synthesis of Benchmark Results, OECD/NEA T-JUNCTION BENCHMARK, 2010.

T-junction thermal mixing flow #2

Time averaged values for U - (a) and W – (b) versus z/R at x/D=1.6.



A coincidence of numerical predictions and experiment is satisfactory.

Failure to take account of some effects and usage of a rough grid are responsible for the observed divergence.

RMS of the velocity x (c) and z (d) component fluctuations versus z/R at x/D=1.6.



T-junction thermal mixing flow #3



Frequency (Hz)

SIBERIA Experiment (Kutateladze Institute of Thermophysics)



- The assembly is designed as a closed hydrodynamic circuit with operating fluid thermal stabilization system. Working area is a plexiglas vertical tube of inner diameter of D= 42.2 mm and L= 3,600 mm.
- Sensors are mounted on inner metal tube with outer diameter d = 20 mm. Equivalent diameter of annular channel is D – d = 22.2 mm.

Experiment conditions.

- Ferro- and potassium ferrocyanide and sodium bicarbonate is dissolved in distilled water to make an operating fluid. Physical properties of this solution are similar to water characteristics.
 - The temperature of operating fluid is 25° C. Fluid viscosity corresponds to the one of distilled water under 25° C (10-6 m2/s). Average fluid velocity is 0.55 and 1.1 m/s against flow area of annular channel.

Simulations of flow in the geometry analog of SIBIRIA test facility by means CONV3D

Friction vs angle

Rms friction vs angle



OECD/NEA-MATIS-H BENCHMARK

Schematic of MATiS-H test facility





(a) Split-type spacer grid





This cold loop test facility, with the acronym MATIS-H (Measurement and Analysis of Turbulent Mixing in Subchannels – Horizontal), is used to perform hydraulic tests in a rod bundle array at normal pressure and temperature conditions.

The rig consists of a water storage tank (e), a circulation pump (f) and a test section (a). The volume of the water storage tank and the maximum flow rate of the circulation pump are 0.9 m3 and 2 m3/min., respectively. The flow rate in the loop during operation is controlled by adjusting the rotational speed of the pump, and the loop coolant temperature is also accurately maintained within a range of $\pm 0.5^{\circ}$ C by controlling the heater (*i*) and the cooler (*h*) in the water storage tank.

For monitoring and controlling the loop parameters (flow rate, pressure and temperature), a mass flowmeter (*m*), a gauge pressure transmitter (o) and a thermocouple (n) are installed at the inlet to the test section.

MATIS-H #1:



Average velocities and RMS are presented in the cross planes at $z/D_H=0.5$, 1.0, 4.0, 10.0 from the downstream face of the spacer grid (measurement section A-A), where. D_H =24.27mm.

All the results are measured along of the three line segments in a ¼ section, namely at y1= 16.56 mm, y2=49.68 mm and y3=81.29 mm marked in red in Figs. 1.





A-A Section

Average velocity U at y=16.56mm

MATIS-H#2:



MATIS-H #3:____ Rms U velocity at y=16.56mm



MATIS-H #4:____ Average velocity V at y=16.56mm



MATIS-H #5:___ Rms V velocity at y=16.56mm



SOCRAT-FR Development

Integral Code SOCRAT-FR is developing on the basis of SA code SOCRAT certified for VVER NPPs

Goals:

Safety justification of the new generation SFR (FR-800, FR-1200)

Application Field:

Numerical modeling of SFRs behavior under BDBA conditions from initial set of events up to release of FP to environment.

Multi-physics BE SOCRAT-BN code structure



The current state of SOCRAT-BN code development

Directions of development	The current state
Closing equations and thermo-physical properties for sodium coolant.	Implemented. Verification
Non-condensable gases transport.	Implemented. Verification
3-d diffusion neutronics module	Implemented. Debugging and assessment.
Improvement of severe accident module SVECHA for SFR core degradation modeling in course of SA.	Implementation of fuel and cladding properties Melt relocation model assessment.
FP transport to the environment (NOSTRADAMUS code).	Implementation.

The prospects of development integral code SOCRAT-BN

Directions of development	The prospects
Aerosols and FP transport in NPP building (updating KUPOL code - IPPE).	Integration to SOCRAT-BN
FP generation in the fuel and FP release to coolant.	Integration to SOCRAT-BN
Thermo-mechanics of fuel rods (transients and accidents).	Integration to SOCRAT-BN
FP and corrosion products transport by coolant and their settling on the construction elements.	Integration to SOCRAT-BN

Verification matrix of thermal-hydraulic model code SOCRAT-BN

Country, laboratory, facility	Type of experiment	
Italy, JRC Ispra, ML-4	Determination of the pressure drop in stationary boiling experiment in tubular geometry	
	Determination of the pressure drop in stationary boiling experiment in annular geometry	
Germany, KNS	Heat transfer in steady and unsteady boiling in 37-pin bundle	
Germany, NSK	Dynamic boiling tests in tubular channel (coolant flow rate was lowered by linearly)	
	Simulation of loss-of-flow (LOF) experiments (coolant flow rate was lowered by linearly)	
Japan, SIENA	Simulation of loss-of-flow (LOF) experiments (coolant flow rate was lowered by hyperbolically)	
USA, ANL, SLSF	Simulation of loss-of-flow (LOF) experiments (coolant flow rate was lowered by hyperbolically)	
USA, THORS Oak Ridge National Laboratory	Sodium boiling in a blocked LMFBR subassembly	
USA, FFM	Sodium boiling in a blocked LMFBR subassembly (19-pin bundle)	
Russia, IHT RAS	Determination of the pressure drop and heat transfer in boiling experiment in tubular geometry	

Two-phase sodium flow in channel with induction heating

Test-section scheme Nodalization scheme P = 1 Bar CHANNEL 300 BOUNDARY Test facility ML-4, EAT ELEMENT Italy, JRC Ispra 240 TRANS DUCER 140 ΔP measured pressure drop Out1 đ T200 C Þ٥ T240 흉 12, 21 200 20 P_IN 19 CH3 18 17 16 heating zone Δ=1,315M 15 14 ΔP 13 12 11 10 0 명 Heat 20 5 P_OUT 8 . 뵹 380 Ø = 6.0×29 In1

Two-phase sodium flow in channel with induction heating

Pressure drop in channel



Heat transfer in liquid sodium (heated annular channel)

Test-section scheme

Nodalization scheme



Heat transfer in liquid sodium (heated annular channel)

Calculation results









Sodium boiling in 7-pin bundle



Nodalization scheme

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Sodium boiling in 7-pin bundle

Experiment conditions



SOCRAT-FR Verification on BN-600 data

Scheme BN-600 (LMFR type)

Primary circuit nodalization



Transient results

Coolant temperature



inlet core sodium temperature

inlet and outlet IHX sodium temperature

Varia: tool for multivariate simulation

Varia performs following tasks:

- Creates the directory tree
- Creates modified input decks and controls launching of the instances of the BE code
- Performs distribution of the instances between computational units
- After the termination of all instances a statistical assessment of the results is performed



SOCRAT/HEFEST code

SOCRAT – System Of Codes for Realistic AssessmenT of severe accidents HEFEST – Highly Efficient Finite-Element Solution for Thermal problems



Impact of heat redistribution: melt retention for generic VVER-1000

Maximum sidewall heat flux



Maximum sidewall heat flux < 600 kW/m²
Maximum flux depends on Zr oxidation

In-vessel melt retention: thermal mechanics (HEFEST-M code)

Long-term strength model was validated on LHF (Sandia labs) experiments

Creep parameters are considered

 $\sigma_{y}(T, d^{p}, \varepsilon^{p}) = \sigma_{y}^{0}(T) + E_{t}(T)\varepsilon^{p} + f(d^{p}, T)$

 $f(d^p,T) = B(T)(d_p)^{\beta}(T)$

cto

The

- Temperature field and vessel melting from previous simulation (highest flux)
- 130 code instances (0.95/0.99)



Varied parameters

Varied parameter	Range
В	$\pm 20\%$
β	± 5%
Long-term strength parameter	± 30%

Filippov A.S., Drobyshevsky N.I., Strizhov V.Th., Simulation of Vessel-with-melt Deformation by SOCRAT/HEFEST Code, 17th Int. Conf. on Nucl. Eng., ICONE17, July 12-16, 2009, Brussels, Belgium

In-vessel melt retention: thermal mechanics (HEFEST-M code)



After 200 000 s (more than 2 days) the residual thickness exceeds 3 cm.

Min	Max	Average
3.4 cm	6.1 cm	5.1 cm



What will happen in longer timespan?

Heat flux will decrease and:

- In metallic layer RPV thickness will increase
 - In oxide layer heat-insulating crust will grow and T will decrease

Summary

Advanced CFD codes allow predictions of local flow characteristics

Computation technique realized in the CONV3D was tested on HPC and showed effectiveness of algorithms for parallel computations

Integrated best estimate multi-physics tools based on simplified description of processes can be used in combination with uncertainties evaluation (BEPU methoodology).