Modelling SEALER with Serpent and OpenFOAM

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Outline

- Introduction
- SEALER
- OpenFOAM
- Multi-physics interface in Serpent 2
- Serpent model
- OpenFOAM model
- Coupling
- Results of test calculation
- Challenges

Introduction

- Coupled neutronics/thermal-hydraulics problem
  - Neutronics with Serpent (power distribution)
  - Thermal-hydraulics with OpenFOAM based CFD solver (density and temperature distributions)
  - MC neutronics + CFD = high fidelity
- The coupled problem is solved by iterating between Serpent and OF solver
- External coupling: All information between the two codes is transferred using OpenFOAM field files
- The coupled code system is used to simulate SEALER in steady state at full power

SEALER (Swedish Advanced Lead Reactor)

- 8 MWt (3 MWe) small lead-cooled fast reactor designed by LeadCold Reactors
- 19.9 % enriched UO_2 fuel
- No refuel during the lifetime of the reactor (~30 years)
- Designed for commercial power production in remote, off-grid sites
- Cooled with forced convection of lead during normal operation
- In emergencies, decay heat can be removed passively with a combination of natural convection of lead and radiation through the reactor vessel

http://www.leadcold.com/images/primarysystemnoconcrete-268.jpg

OpenFOAM

- Free, open source C++ toolbox for continuum mechanics problems, including CFD distributed by the OpenFOAM Foundation
- Includes a large library with many functionalities such as tensor and field operations, discretization, mesh, solution to linear equations, turbulence models etc.
- Also approximately 250 ready made applications including solvers, and tools for meshing and pre- and post-processing
- OpenFOAM 4.x was used in this work
- OpenFOAM is freely available at openfoam.org

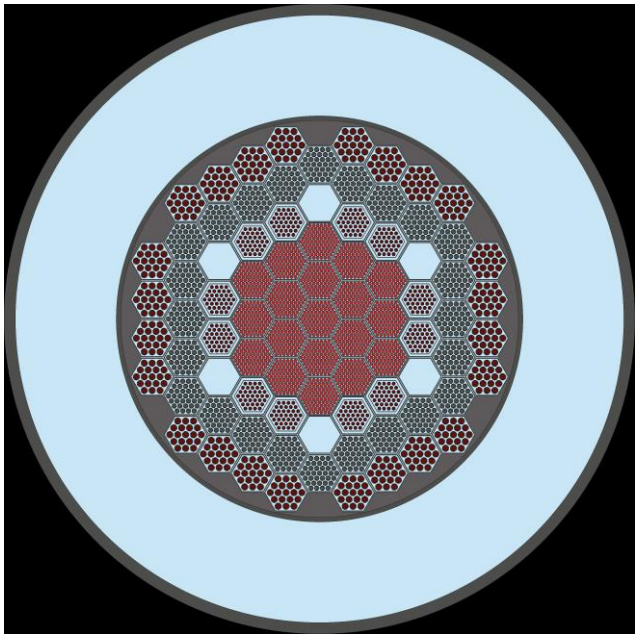
Multi-physics interface in Serpent 2

(See: Multi-physics interface at Serpent Wiki)

- Allows the modelling of materials with arbitrarily refined temperature and density distributions supplied by an external solver
- Supports several formats, one of which is based on the OpenFOAM unstructured mesh format (See: Wiki page)
- The same format can also be used to pass the volumetric power density to the external solver
- From the user point of view easy to use as one can pass the temperature/density/power distribution without modification from one code to another
- Geometry can also be defined based on the OF mesh (See: Wiki page)

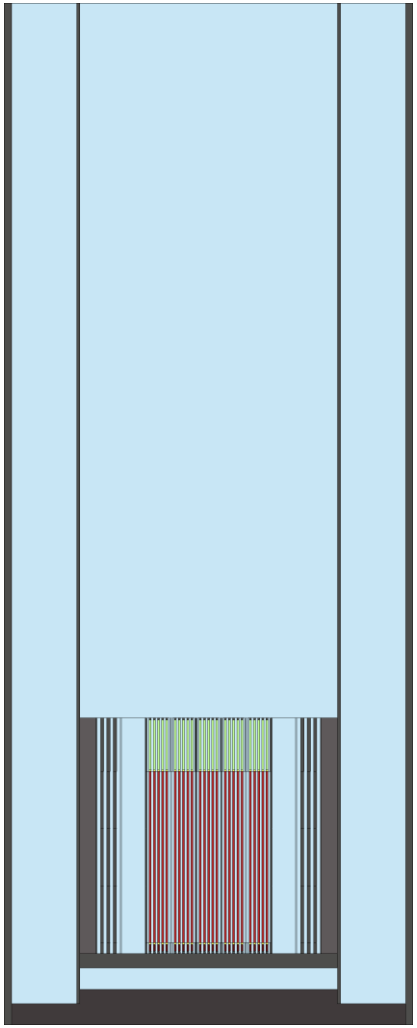
Serpent model (1/2)

- Provided by LeadCold Reactors
- 1/6 symmetry of the core is utilized with the universe symmetry option (See: Wiki1, Wiki2)
- Core configuration:
  - 19 fuel assemblies each containing 91 fuel rods
    - Height of the fuel column 1200 mm
  - 12 control assemblies
  - 6 shutdown assemblies (withdrawn in the picture)
  - 24 reflector assemblies
  - 24 shield assemblies
  - All assemblies are wrapped by hex-cans



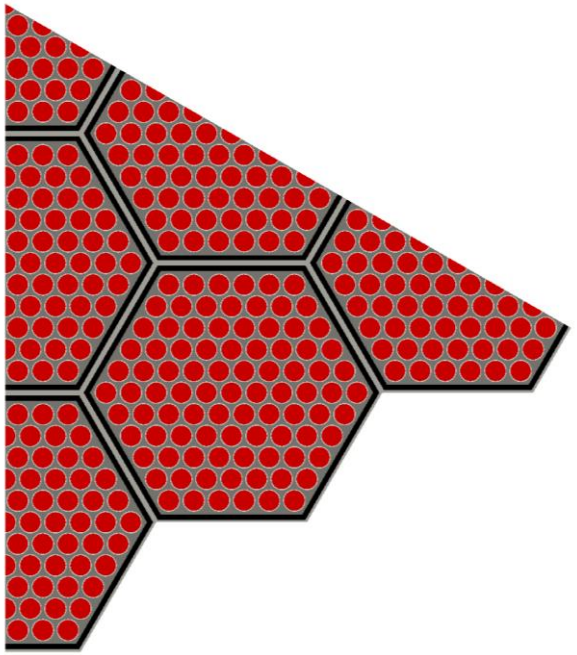
Serpent model (2/2)

- Active axial region of the fuel assemblies is linked to the multi-physics interface
- Separate interface definition file for each material in this region (fuel, cladding, hex-cans, lead)
- Fuel (UO_2), cladding (D9), hex-cans (D9): constant densities, only temperature distributions from OF
- Lead: density and temperature distributions from OF
- Power is tallied directly on the fuel mesh with each cell as a separate power tally bin
- Total fission power is set to 8 MW



OpenFOAM model (1/3)

- Conjugated heat transfer problem is solved with a modified version of chtMultiRegionSimpleFoam
- 1/6 of the fuel assemblies is modelled with symmetry boundary condition at radial boundaries
- Five regions (each with own mesh)
  - Solid: fuel, cladding, hex-cans
  - Fluid: lead inside the fuel assemblies, lead in the gaps
- Connected with a custom boundary condition that balances heat flux calculated using enthalpy on the boundaries
  - Simple gas gap model to add thermal resistance to the fuel-cladding interface
- Meshes were generated with ANSYS Fluent Meshing and OF tools (~27 million cells in total)



OpenFOAM model (2/3)

- Laminar flow in the gaps between assemblies
- Turbulent flow inside fuel assemblies
  - k-ω SST turbulence model with wall functions
  - New thermal wall function for low Prandtl number flows[1)]
  - Variable turbulent Prandtl number based on Kays correlation[2)]
- Thermophysical properties for different materials (liquid lead[3)], D9[4)], UO_2[5)]) were implemented to OpenFOAM
- A custom fvOptions source to import the volumetric heat source from Serpent

1) M. Duponcheel et al. “Assessment of RANS and improved near-wall modeling for forced convection at low Prandtl numbers based on LES up to Re =2000.” International Journal of Heat and Mass Transfer, volume 75(Supplement C), pp. 470 – 482 (2014).
2) W. M. Kays. “Turbulent Prandtl number–where are we?” Journal of Heat Transfer, volume 116(2), pp. 284–295 (1994).
3) C. Fazio et al. “Handbook on Lead-bismuth Eutectic Alloy and Lead Properties, Materials Compatibility, Thermal-hydraulics and Technologies-2015 Edition.” Technical report, Organisation for Economic Co-Operation and Development (2015).
4) L. Leibowitz et al. “Thermal Conductivity and Thermal Expansion of Stainless Steels D9 and HT9*.” Technical report, Argonne National Laboratory (1988).
5) W. Luscher et al. “Material property correlations: Comparisons between FRAPCON-4.0, FRAPTRAN-2.0, and MATPRO.” Technical report, Pacific Northwest National Laboratory (2015).

OpenFOAM model (3/3)

- Inlet temperature: 663 K
- Total lead mass flow: 1300 kg/s
- Exact inlet velocity distribution is not known
- Calculating the inlet velocity distribution would have required an additional CFD calculation and information such as the core orificing which was not available
- Simplications were made:
  - Fully developed flow at inlet
  - 1 % of the total mass flow was allocated to the gap
  - Rest of the mass flow was allocated to assemblies based on assembly-wise powers from an uncoupled Serpent calculation

Coupling

(See: Coupled multi-physics calculations at Serpent Wiki)

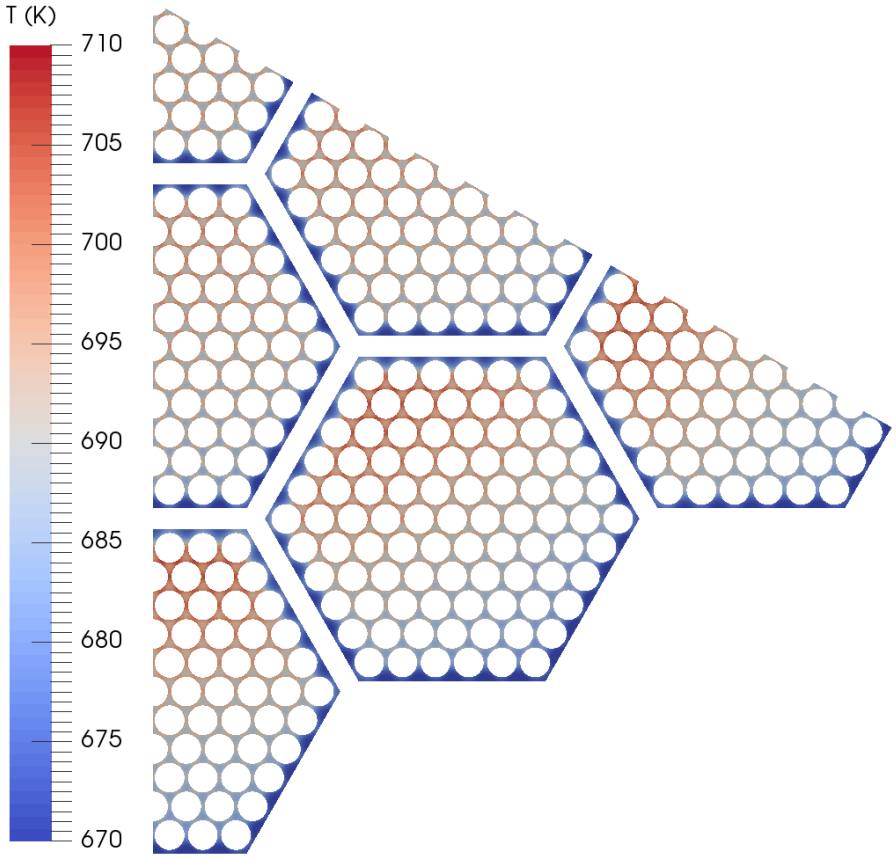
- Coupling program written in Python was used to run Serpent and OF solver in turns
- OF solver is restarted on each iteration
- Serpent communicates with the coupling program using POSIX-signals
- The temperature/density/power distribution data is transferred between the codes using OF field files
- Iteration is started with a Serpent calculation with uniform temperature and density distributions in the regions modelled with the OF solver
- Stochastic nature of the Monte Carlo neutronics poses a convergence challenge in the coupled calculations
  - Always some statistical uncertainty in the fission power distribution
  - To tackle this problem a relaxation scheme based on stochastic approximation scheme is applied (See: Wiki page)

$$P_{\mathrm{rel}}^{(n+1)} = \left(1 - \frac{1}{n+1}\right) P_{\mathrm{rel}}^{(n)} + \frac{1}{n+1} P^{(n+1)}$$

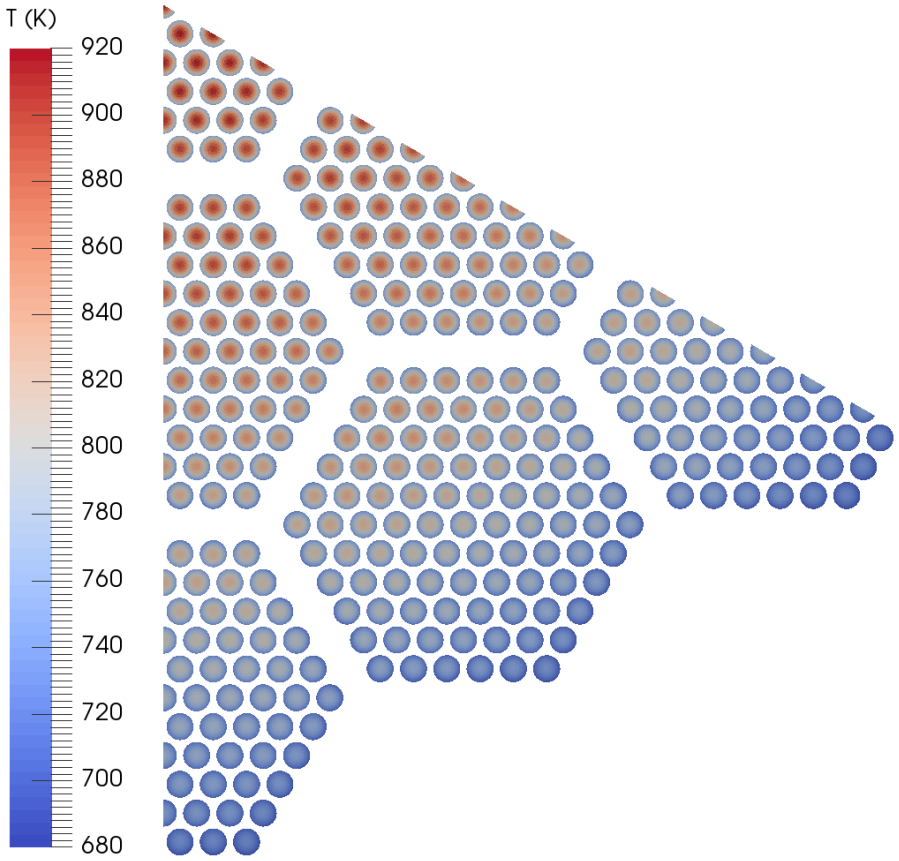
Results of test calculation (1/2)

- Coupled calculation was run for 8 iterations
- Total calculation time ≈ 160 h on a node with two Fourteen-Core Intel Xeon E5-2697 v3 2.6 GHz processors with 128GB RAM memory
  - On each iteration Serpent simulation took ~12 h
- At each coupled iteration 1e9 active neutron histories divided into 1000 cycles of 1e6 neutrons were simulated
- On the first iteration 50 inactive cycles and on the following iterations 30 inactive cycles were run
- Fission source passing was used (See: Wiki page)
- Convergence was evaluated retrospectively by comparing fuel temperature distributions on two consecutive iterations
  - Already after the second iteration the maximum difference was only $\Delta T \approx 1.4\ \mathrm{K}$

Results of test calculation (2/2)



Lead coolant temperature



Fuel temperature

Challenges (1/4)

- Serpent and OpenFOAM geometries don’t fully agree
  - CSG geometry model in Serpent vs. OpenFOAM unstructured mesh based geometry
  - Differences mostly seen at curved surfaces such as the outer surface of a fuel pellet
  - The amount of differences depend on how the OpenFOAM mesh is generated
- Especially problematic if the power is tallied using OpenFOAM mesh
  - In the current SEALER mesh, the volume of the fuel is approximately 0.36 % smaller than in the Serpent geometry
  - 0.5 % of the thermal power is not tallied to the OpenFOAM cells
  - The sum of individual cell powers was scaled in OpenFOAM to match the thermal power defined in the Serpent input

Challenges (2/4)

- Huge number of power tally bins results in poor statistics
- In the test calculation each OpenFOAM cell had a separate power tally bin -> nearly 9 million power bins
- With 1e9 simulated neutron histories the maximum relative error on the bins was 29 %
- Decreasing the maximum error for example to less than 1 % is not possible with the current computational resources
- One way to decrease the maximum error is to combine individual mesh cells to larger bins containing several cells
- Does the relative error need to be below 1 % in all of the bins as some of the bins have very small volume and/or power?
- In general, the modelling of fuel rods with OpenFOAM contains many approximations
    - Separate fuel performance code and only fluid flow is solved with OF?

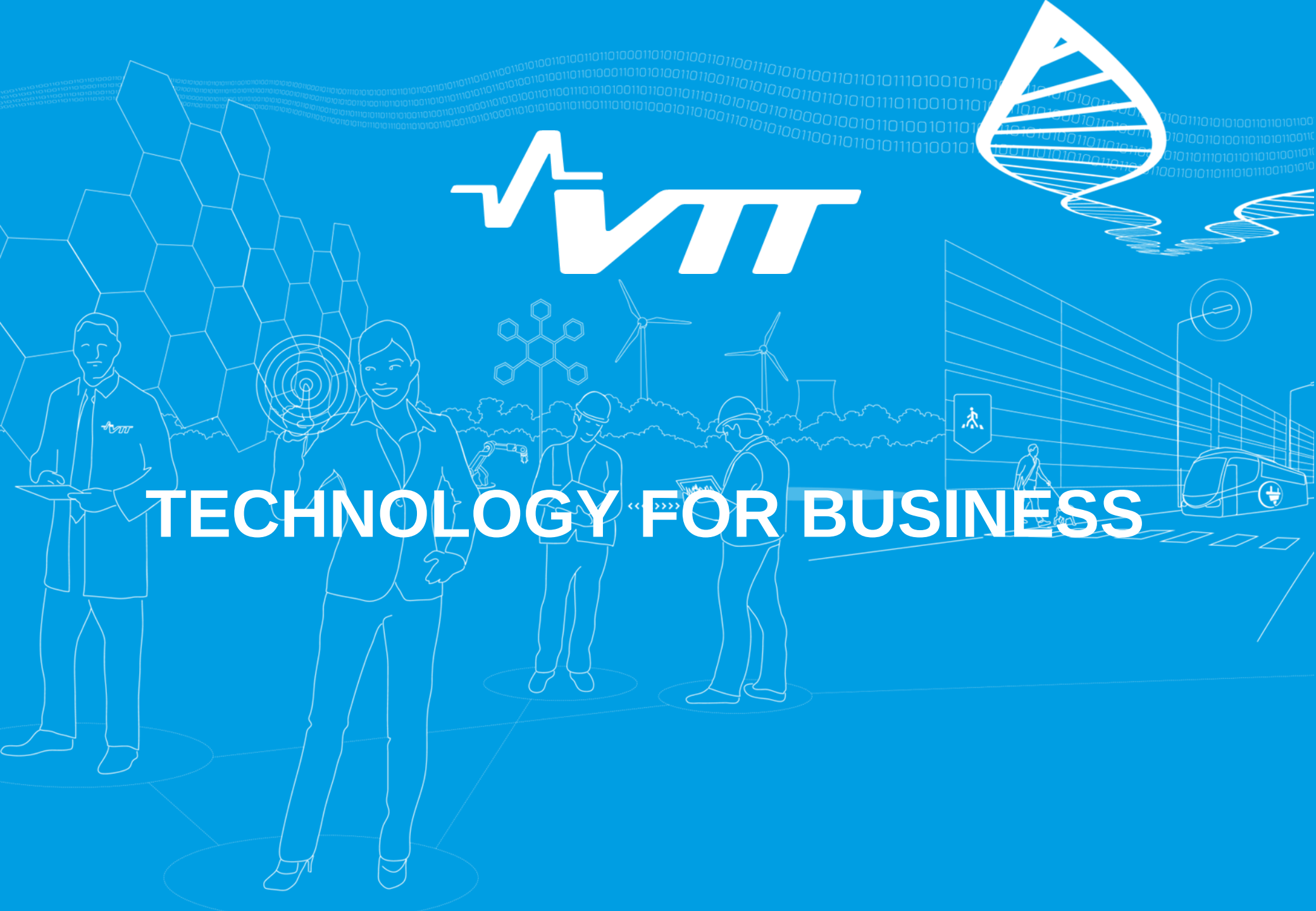
Challenges (3/4)

- In coupled calculations of fast reactors the temperature dependency of unresolved resonance range cross sections should be modelled accurately
- Serpent currently has no option for on-the-fly temperature treatment of unresolved resonance range cross sections
  - The possibility of adding such feature to Serpent should be investigated
- In the coupled test calculation infinite-dilute cross sections were used

Challenges (4/4)

- Numerical simulation of turbulent heat transfer in low Prandtl number flows such as those of liquid metals is a complex issue
- At low Prandtl numbers the classical Reynolds analogy, which assumes similarity in the turbulent transport features of momentum and heat, is generally not valid
- This is a challenge, since the most common way to model the turbulent heat flux in RANS simulations is based on the Turbulent Prandtl number concept which relies on the similarity assumption
- In the test calculation the Turbulent Prandlt number concept is used regardless of its shortcomings
  - Accuracy of the CFD calculations is not known

Thank you! Questions?
Ideas?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