Kraken – the new platform for reactor simulations at VTT

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Background and goals

Finnish nuclear legacy is still very much alive at VTT ⇒

```
C       Control words
        IF (L .GT. 0) GO TO 270
   70   IF (J .LT. 80) GO TO 80
        ASSIGN 80 TO RD
        GO TO 820
   80   J = J + 1
        IF (CM(J:J) .EQ. ' ') GO TO 70
        DO 90 I = 1,10
   90   MX(I) = 32
        I = 1
  100   IF (CM(J:J) .EQ. MASK1(1:1)) GO TO 120
        MX(I) = M(J)
        IF (J .LT. 80) GO TO 110
        ASSIGN 110 TO RD
        GO TO 820
...
```

Kraken will serve as the renewal of

1. simulation chain: Calculation codes.
2. expertise: The people using the codes.

Goals:

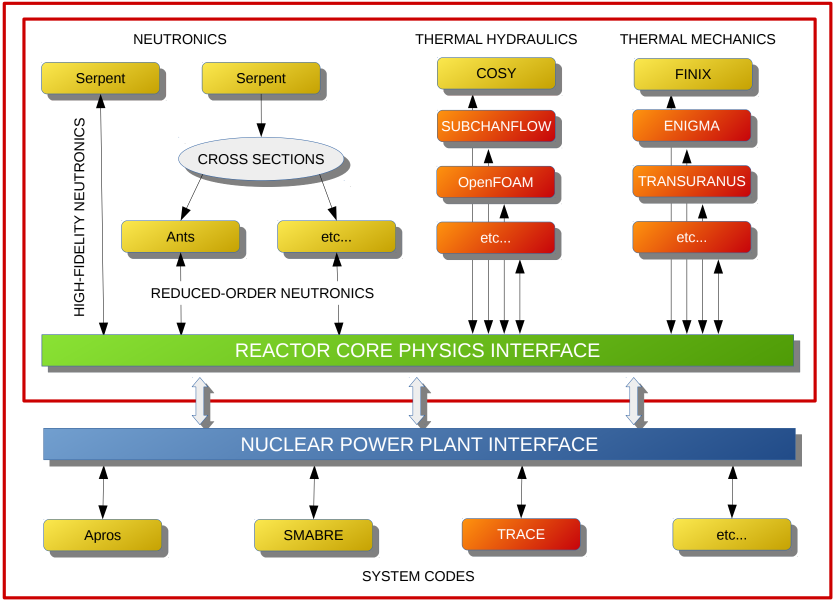
Build expertise from source-code level knowledge.

Engage/commit young experts at VTT through the development and use of their own code(s).

Approach:

Leverage the existing Finnish tools. Kick-start the creation of new ones.

Couple to state-of-the-art tools from abroad.


NEUTRONICS
THERMAL HYDRAULICS
THERMAL MECHANICS
Serpent
Serpent
COSY
FINIX
SUBCHANFLOW
ENIGMA
CROSS SECTIONS
OpenFOAM
TRANSURANUS
HIGH-FIDELITY NEUTRONICS
Ants
etc...
etc...
etc...
REDUCED-ORDER NEUTRONICS
REACTOR CORE PHYSICS INTERFACE
NUCLEAR POWER PLANT INTERFACE
Apros
SMABRE
TRACE
etc...
SYSTEM CODES

General plans

Kraken will slowly take over as the main reactor analysis tool at VTT.

The codes developed for the Kraken platform need to have flexibility in order to model any reactor type (Gen II, Gen III(+), Gen IV).

Development of in-house codes is complemented with couplings to existing state-of-the-art solvers.

The flexible fidelity approach taken means that the different physics (neutronics / TH) can switch between a high-fidelity and a reduced order solver as needed.

The main development tasks include:

- Development, verification and validation of separate solvers.
- Coupling of the solvers to a multi-physics solver.
- Verification and validation of the coupled solution.
- Design and implementation of an effort-saving front-end for pre-processing and post-processing.

Reduced-order calculation sequence

Reduced order methods rely on the conventional multi-stage calculation scheme and spatial homogenization.

Nodal diffusion codes are the “workhorses” applied to routine fuel cycle simulations and transient safety analyses.

Several widely-used codes (Simulate, PARCS, DYN3D, etc.) have been succesfully applied for this purpose for decades.

Approach in Kraken:

- Group constant generation using Serpent
- New AFEN/FENM-based nodal diffusion solver “Ants”, capable of handling square and hexagonal geometries and steady-state and transient solutions
- Other reduced-order methods will be studied in the future

The continuous-energy Monte Carlo method can also be used to provide the ideal reference solution for verifying the reduced-order methodology.

High-fidelity calculation sequence

High-fidelity methods apply a direct solution to the heterogeneous neutronics problem, without spatial homogenization or other intermediate steps.

The methods are computationally too heavy for routine design and safety analyses, but can be used for some specific best-estimate type calculations and validation of reduced-order methods.

High-fidelity multi-physics calculations were extensively studied in the SA-NUMPS project in 2012-2016:

- Direct coupling of Serpent to thermal hydraulics, CFD and fuel performance codes
- State-point information passed via a universal multi-physics interface
- Coupling successfully established with OpenFOAM, Finix and Enigma

The development of the high-fidelity sequence continues where the NUMPS project was left off, and the same interfaces and coupling algorithms will be used with the reduced-order sequence.

High-fidelity methods have been extensively studied within the Serpent user community as well.

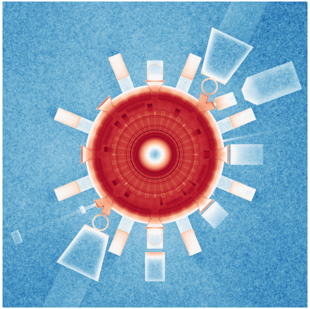
What is it good for?

The objective is that the new computational framework could eventually handle all core physics calculations carried out at VTT either independently or coupled to system codes.

Example applications:

- 3D transient safety analyses and fuel cycle simulations for large LWR cores (PWR, BWR and VVER) using the reduced-order sequence
- Full core calculations for SMR's and small research reactors using both high-fidelity and reduced-order methods
- Research projects involving Gen-IV reactors
- Educational use at universities
- Specific applications that require unconventional methodologies
- Production of source terms for severe accident, radiation shielding and final disposal analyses

What is it good for?



There are also various transport applications in which a coupled solution is not necessarily required:

- Criticality safety
- Radiation transport
- Fusion neutronics
- Modeling of low-power research reactors

These applications often involve complicated and irregular geometries that can only be handled using Monte Carlo particle transport codes.

Serpent has a lot of potential for these applications, and development of Kraken strongly supports these efforts.

Solvers and potential solvers

Reactor physics

High fidelity:

- VTT: Serpent. **2004** –

Reduced order:

- VTT: Ants (AFEN/FENM nodal diffusion), **2017** –
- VTT: Collision probability ROM, **2017** –
- VTT: Point-kinetics ROM for system code coupling, **20xx** –

Serpent is used to generate input data for the Reduced Order Models (ROMs).

Developing both steps of the two-step chain in-house is one main ingredient in obtaining excellent results (see, e.g. CASMO-SIMULATE).

Fluid mechanics

High fidelity:

- Ext/VTT: OpenFOAM CFD.

Reduced order:

- VTT: COSY (coarse mesh porous flow), **2012** –
- VTT: Kharon (closed channel steady state coarse mesh porous flow), **2017** –
- Ext/VTT: OpenFOAM (coarse mesh channel/subchannel level solver, open channel, steady state/transient)
- Ext: SUBCHANFLOW (KIT)

OpenFOAM is one of the main tools used for CFD modelling at VTT. The source code level understanding for OpenFOAM is achieved through the implementation of new models and solvers.

Fuel performance and thermal mechanics

High fidelity:

- Ext: BISON? (MOOSE)
- Ext: OpenFOAM?

Reduced order:

- VTT: FINIX (1.5D fuel performance, steady state, transient, irradiation), **2012** –
- Ext: ENIGMA (BNFL, 1.5D fuel performance)
- Ext: FRAPCON/FRAPTRAN (U.S.DOE, 1.5D fuel performance)
- Ext: TRANSURANUS (EU, 1.5D fuel performance)

Thermal mechanics solvers need to be written separately for non-fuel pin deformations, which can be quite important in some Gen IV concepts.

System codes / power plant simulators

- VTT: Apros **1986** –
- VTT: SMABRE **early 1980's** –
- Ext: TRACE (Purdue University & U.S.NRC).

Apros and SMABRE share the same thermal hydraulics model. TRACE will most likely be used in Finland as an independent modeling tool (diversity principle of nuclear safety).

System codes will connect to Kraken through a separate power plant interface.

Coupling approach

Coupling approach

Hub-and-spoke approach for data transfer means that each code only needs to interface with the multi-physics driver.

Multi-physics driver needs to understand every single code and how to transform and transfer data between the codes.

Several existing multi-physics platforms/frameworks/models to learn from:

- MOOSE (USA / INL)
- OpenFOAM
- SALOME (EU / CEA, EDF)
- VERA (USA / CASL)

Of these options, the coupling approach in VERA is most likely closest to the one we will be choosing.

Coupling approach

The multi-physics driver needs to accommodate tools with various levels of flexibility:

- New modular solvers that are developed for the computational framework from the start.
- Existing codes developed at VTT that can be easily modified.
- External third-party tools that are somewhat non-flexible in their coupling.

External coupling was chosen as the approach

- The easier approach for single solver developers.
- Also applicable for third-party solvers with no access to the source code.

Data transfer using sockets (no disk I/O).

A fallback option using files.

Coupling approach

One grand goal is to have a common Kraken front-end to ease things such as:

- Calculation setup.
- High-fidelity – reduced order comparisons.
- Uncertainty propagation.

In the beginning, however the user will need to set up each code separately. Initial use cases may point out which specific tasks might be easier to conduct via the Kraken front-end.

The development of the front-end also depends on the funding decisions of larger projects where Kraken or Serpent will be used in educational purposes (e.g. SA-VIRNE, EU-OpERA).

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