Kraken workshop

Introduction to the Kraken framework

Ville Valtavirta

Outline

- Kraken on one slide

- Motivation for Kraken development.
- Overarching development goals.
- Coupling scheme in Kraken.
- Development history and future.

- Licensing and distribution

Kraken

VTT is replacing its legacy reactor analysis toolchains (HEXTRAN, TRAB-3D) with a new set, **Kraken**, building largely on VTT's own modern solvers.

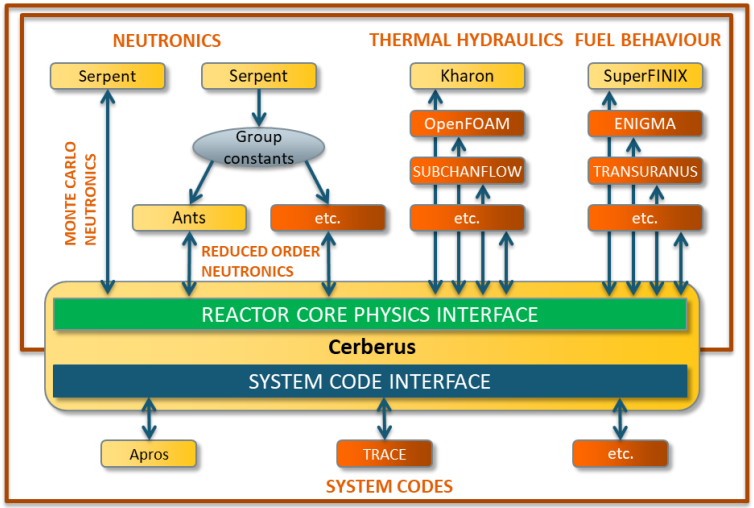
Kraken will provide VTT with the **tools** required for future safety analyses and the **expertise** to use those tools in a proper manner.

Kraken is designed both for **independent determinist safety analyses** and **evaluation of new reactor concepts**.

Basic capabilities for **steady state**, **fuel cycle** and **transient** analyses implemented during 2019-2021.

Validation effort ongoing with focus on demonstrating capabilities required for deterministic safety analyses.

A **non-commercial user license** is being drafted with **international distribution** planned through OECD/NEA data bank and RSICC later in 2022.



A schematic representation of the plans for the completed Kraken framework. Finnish solver modules developed at VTT are shown in yellow, while potential state-of-the-art third party solvers to be coupled are shown in orange.

Background and development goals

Motivation for Kraken development

Historically the independent deterministic safety analyses for Finnish reactors have been conducted by Finnish organizations using Finnish reactor analysis tools.

Many of the tools previously in use at VTT were originally developed in the 80’s and 90’s educating a whole generation of experts into the field of reactor analysis.

The aging of both tools and expertise leads to challenges.

New reactor types (e.g. SMRs) are expected to enter the market.

Recently Serpent development and user community have given some valuable lessons on:

- Active code development providing source code knowledge and motivation for young scientists.
- International user community tackling wider research topics and providing valuable feedback and contributions.

Motivation for Kraken development

Recent work in Serpent development focused on:

- Generating group constants for nodal solvers.
- Coupled multi-physics calculations

Aging legacy codes and experts + new applications (SMRs, HTGRs, …) + good experience from Serpent development

Decision in 2017 to:

Start a project to build Kraken, VTT‘s reactor analysis framework for future **research work** and **safety analyses**.

Provide a non-commercial license for the framework early on so that interested scientists around the world can get involved.

Development goals for Kraken

Kraken aims to be

Capable: Can evaluate fulfilment of design bases according to Finnish YVL-guides and NUREG 0800.

Usable: Offers a reasonable user interface while automating the routine parts of analyses.

Modular: Allows cross-verification of single physics solvers even in coupled transients.

Alive: Maintains source-code level expertise of the different parts of the framework.

Excellent: Uses state-of-the-art and beyond-the-state-of-the-art approaches whenever possible.

Kraken is intended as a

Safety analysis tool, able to conduct Finnish deterministic safety analyses in the future,

Research and design tool that can be applied to reactor core related research problems including the design of new reactor concepts,

Learning and teaching tool to be used in virtual reactor labs and thesis projects / assignments.

Code coupling approach in Kraken

Couplings for coupled calculations

Codes can be coupled in many ways:

- Memory level coupling:

Codes compiled together or linked as libraries. Executed as a single process.

- MPI or socket based coupling:

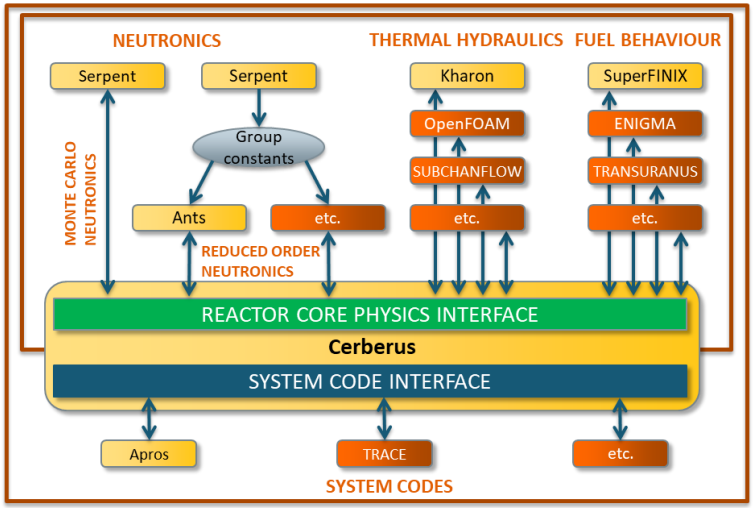
Data exchanged between separate processes using common protocols.

- Input/file based coupling:

External driver updates code inputs based on the outputs of others.

Kraken is intended to bring together solvers from various sources:

- Those developed at VTT specifically for Kraken.
- Those already developed at VTT, not specifically for Kraken.
- Externally developed codes, for which source code may be available.
- Externally developed codes, for which source code is not available.



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Couplings for coupled calculations

A central multi-physics driver Cerberus.

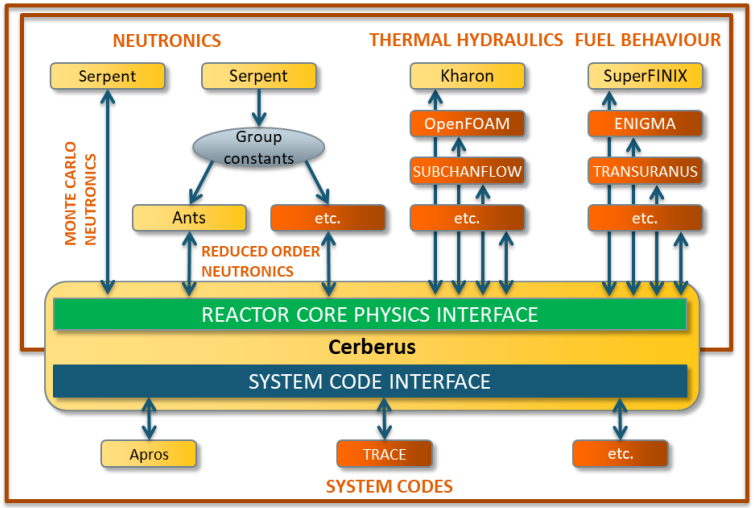
- Each solver only needs to communicate with Cerberus.

Data transfer through sockets.

- Native Kraken solvers support socket communication automatically.
- Others utilize wrapper programs. SCFWrap, TUWrap, TRACEWrap.

Code agnostic and modular coupling approach.

- Cerberus does not know which solver is which.
- All solvers look similar through Cerberus.
- Can exchange solver modules to a higher or lower fidelity easily without changes to other solvers or simulation model as a whole.



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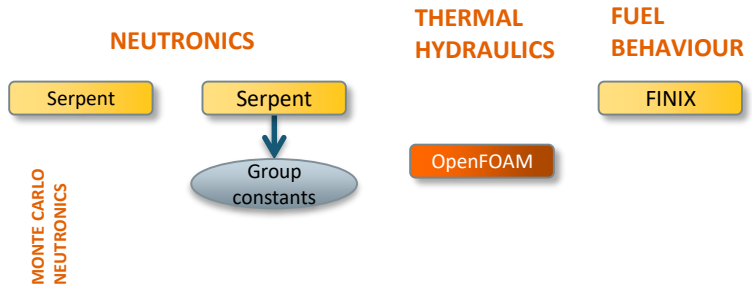
Development history and future plans

Development history and future plans

Pre 2017:

- Serpent developed at VTT since 2004.
- Serpent 2.1.0 in 2012.
- Serpent 2 development focused on:
  - Group constant generation for reduced order solvers.
  - Coupled multi-physics calculations.
- FINIX fuel behaviour solver developed at VTT since 2012.
- VTT participates in OpenFOAM development.

Previous computational framework in use at VTT for deterministic safety analyses.

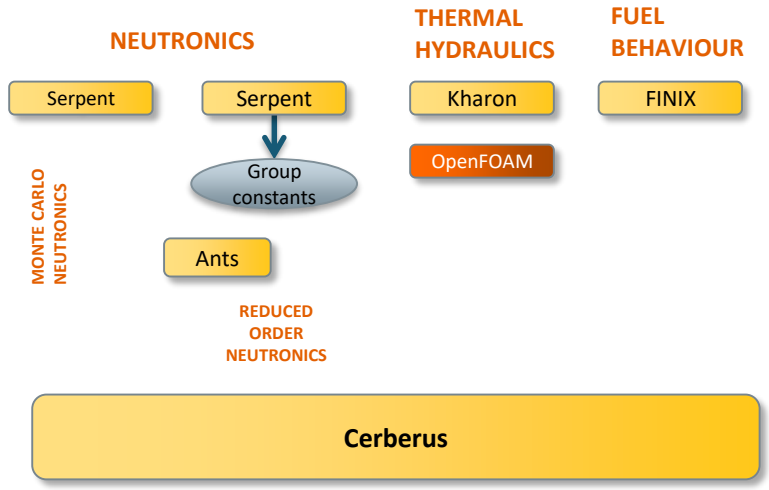


Development history and future plans

2017:

The idea of the renewal of VTT‘s reactor analysis framework and expertise proposed and accepted.

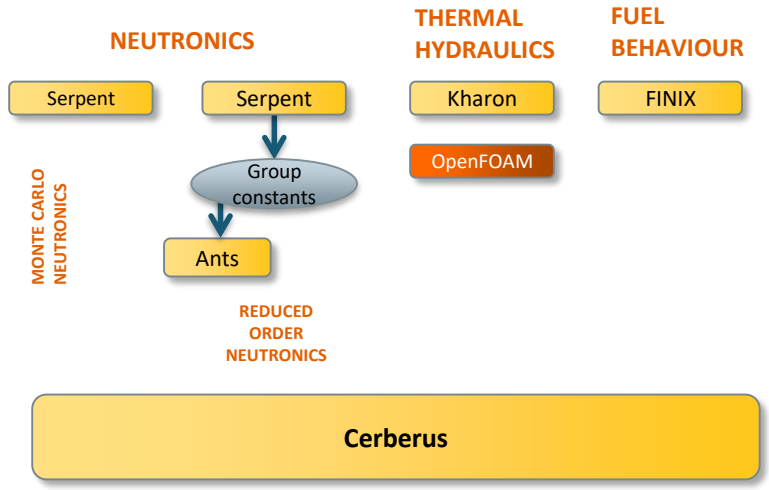
- Development of Ants nodal neutronics program starts.
- Development of the simple two phase closed channel porous medium TH solver Kharon starts.
- First commit in the Cerberus multi-physics driver repository.



Development history and future plans

2018:

- Development work related to Ants.
- Kharon development.
- Drafting plans and project proposals related to large scale Kraken development.



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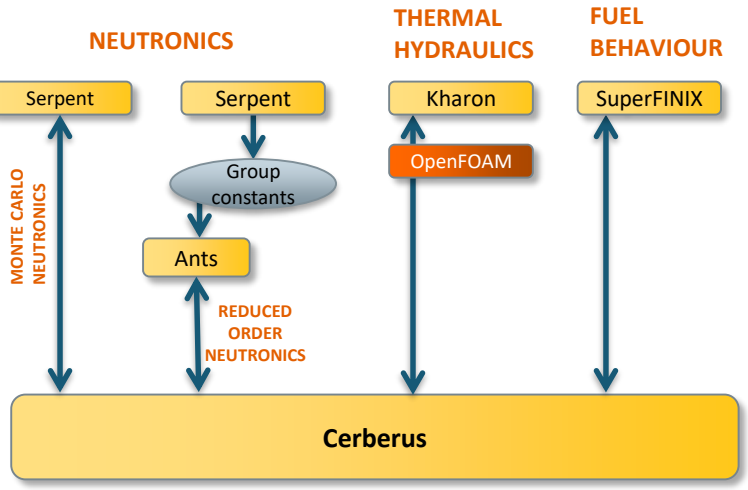
In Proc. 28th Symposium of AER on VVER Reactor Physics and Reactor Safety,
October 8 – 12, 2018, Olomouc, Czech Republic.

Development history and future plans

2019:

LONKERO 2019-2022 project starts.

- SuperFINIX core level fuel behaviour solver created.
- Socket communication syntax established for Cerberus.
- Couplings to several solver modules.
- Coupled steady state calculations (reactivity coefficients etc.)



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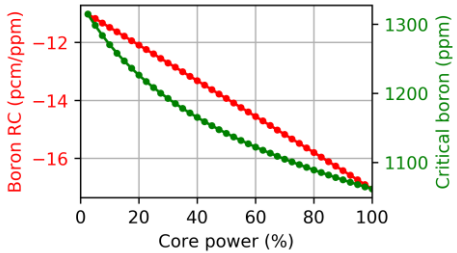
Some work conducted in 2019

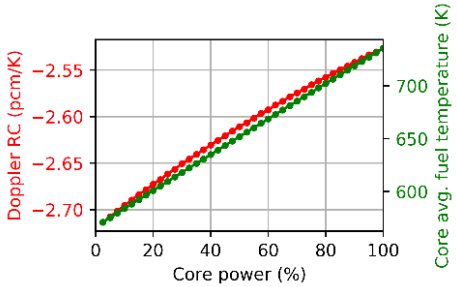
- Demonstrating the **capability** and **modularity** at steady state:

Valtavirta, V., Lauranto, U., Hovi, V., Peltonen, J., Rintala, A., Tuominen, R., Leppänen, J.
"High fidelity and reduced order solutions to an SMR-level progression problem with the Kraken computational framework"
PHYSOR 2020, March 29-April 2, 2020, Cambridge, UK.

	CZP			HZP			HFP		
	Ants	**Serpent**	**A–S**	**Ants**	**Serpent**	**A–S**	**Ants**	**Serpent**	**A–S**
RB1	861	874	–13	1974	2012	–38	2084	2221	–137
RB2	2094	2092	+2	2218	2161	–57	2290	2285	+5
SB3	2592	2597	–5	3547	3559	–12	3612	3697	–85
SB4	2592	2596	–4	3547	3560	–13	3612	3703	–91

Using high-fidelity solver to verify reduced order solver performance also in coupled calculations: Control rod group worths in an SMR core evaluated by Ants and Serpent based coupled calculation sequences in cold-zero-power (CZP), hot-zero-power (HZP) and hot-full-power (HFP) conditions.





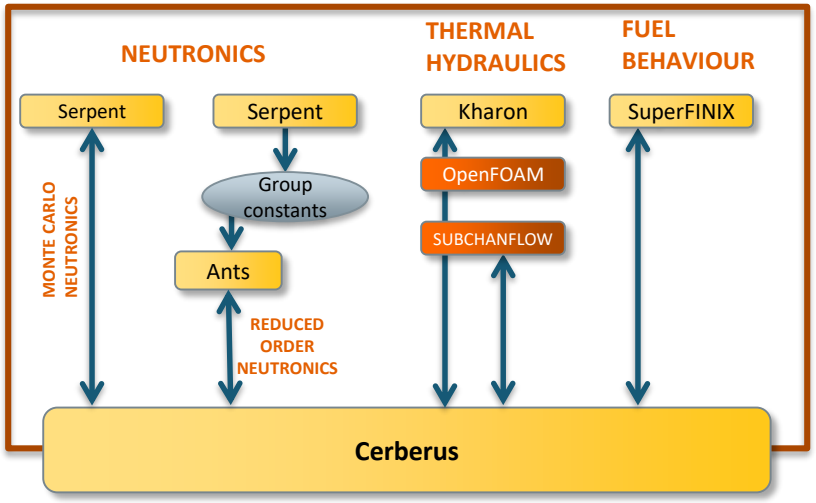
Evaluating licensing relevant data:
Two reactivity coefficients calculated with Ants-Kharon-SuperFINIX for the SMR core at various power levels:
Top: Boron reactivity coefficient (red) and critical boron (green).
Bottom: Doppler reactivity coefficient (red) and core average fuel temperature (green).

Development history and future plans

2020:

Moving from steady state to operating cycle analyses.

- Burnup capabilities implemented.
- A separate reactor simulator Python module automates fuel cycle analyses.
- Coupling SUBCHANFLOW through SCFWrap.



Unna Lauranto
Developing a generic Python based group constant library generator module for Serpent
Special Assignment Report, PHYS-E0441, Aalto University, School of Science, Department of Applied Physics, 2020.

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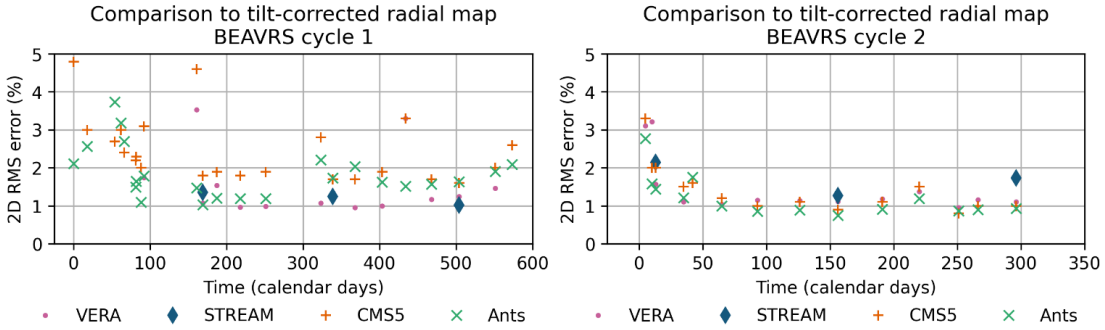
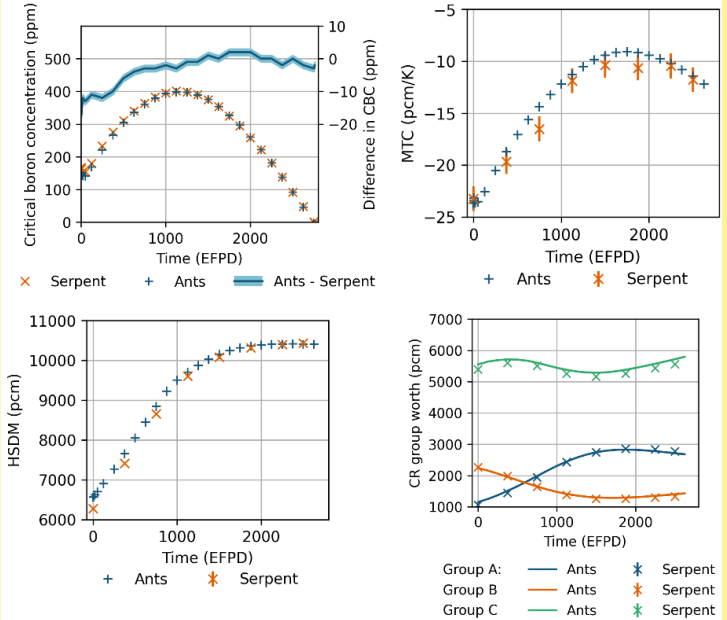
Some work conducted in 2020

- Demonstrating the **capability**, **usability** and **modularity** of the core simulator in operating cycle analyses.
- Beginning the validation of the framework for operating cycle analyses.

Valtavirta, V., Tuominen, R.
A simple reactor core simulator based on VTT's Cerberus Python package
M&C 2021, April 11-15, 2021, Raleigh, NC



Validation: 2D RMS errors when comparing calculated results to measured detector maps during the two operating cycles of the BEAVRS benchmark. Various industry and scientific leaders and Kraken (Ants).



Automatic evaluation of licensing relevant data during the simulation of an SMR operating cycle. Verification by switching one physics from reduced order solver (Ants) to a high-fidelity one (Serpent), while Kharon and SuperFINIX models are kept constant

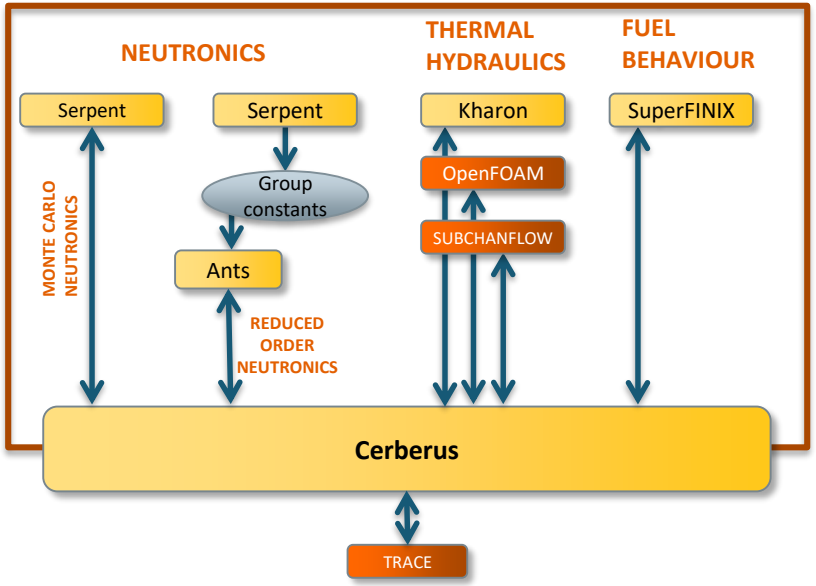
Top left: Boron letdown curve.
Top right: Moderator temperature reactivity coefficient.
Bottom left: Instantaneous hot shutdown margin.
Bottom right: Control rod group worths.

Development history and future plans

2021:

From operating cycle analyses to transient calculations.

- Coupling to TRACE via TRACEWrap and ECI.
  - Paper in this conference by Riku Tuominen (Coupling TRACE with Nodal Neutronics Code Ants Using the Exterior Communications Interface and VTT's Multi-Physics Driver Cerberus)
- Initial coupling to OpenFOAM.
- Begin drafting a non-commercial license.



Valtavirta, V., Tuominen, R.
A simple reactor core simulator based on VTT's Cerberus Python package
M&C 2021, April 11-15, 2021, Raleigh, NC

Hirvensalo, M., Rintala, A., Sahlberg, V.
Triangular geometry model for Ants nodal neutronics solver
M&C 2021, April 11-15, 2021, Raleigh, NC

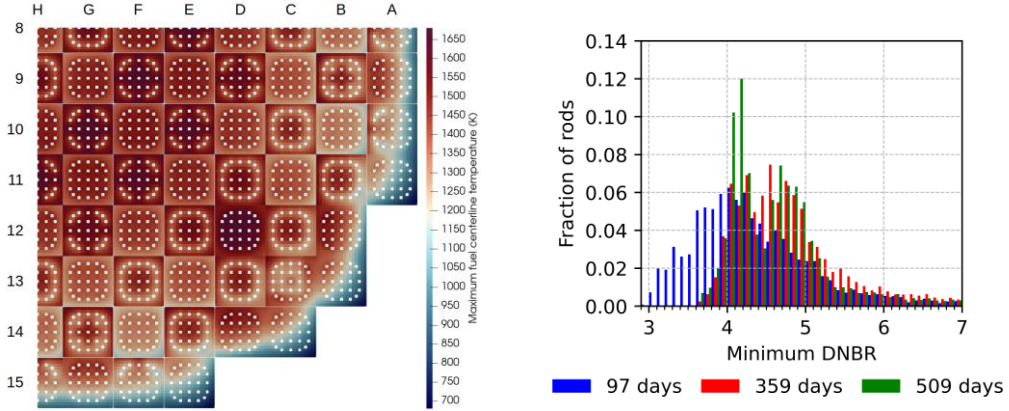
Markus Hirvensalo
Runtime optimization of SuperFINIX multi-rod fuel performance program
M.Sc. Thesis, Department of Applied Physics, School of Science, Aalto University.

Rintala, A., Valtavirta, V., Leppänen, J.
Microscopic cross section calculation methodology in the Serpent 2 Monte Carlo code
Annals of Nuclear Energy 164 (2021)

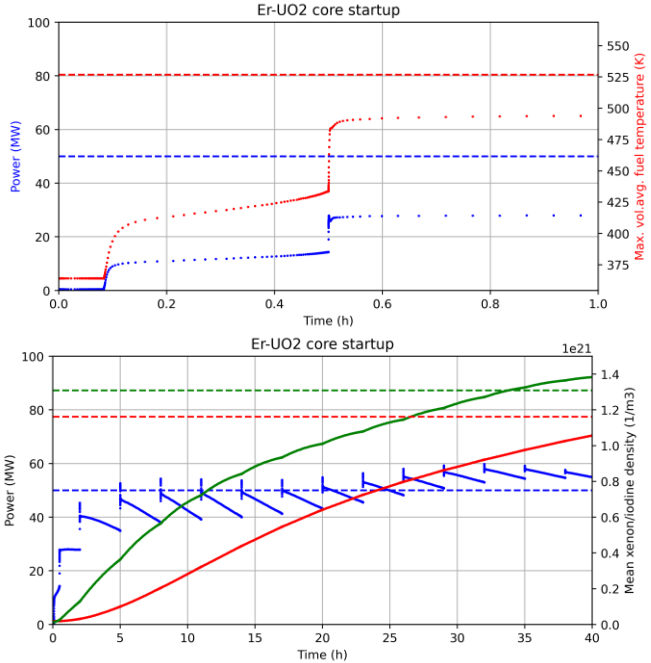
Valtavirta, V., Rintala, A., Lauranto, U. "Validating the Serpent-Ants Calculation Chain Using BEAVRS Fresh Core HZP Data"
Journal of Nuclear Engineering and Radiation Science (2021),

Some work conducted in 2021

- Extending the solvers and coupled solution to **time dependent simulations**.
- Verification of Ants neutron kinetics and dynamics.
- Verification of the Serpent-Ants chain in hexagonal lattice neutronics.
- Advanced methods for in-line thermal margin evaluation.



Rod resolved operating cycle analyses: PWR operating cycle modelled with Ants (pin power reconstruction) - SUBCHANFLOW (subchannel resolved) - SuperFINIX (rod resolved): **Left:** Maximum fuel centreline temperatures at 97 days. **Right:** Rod minimum DNBR distributions at 97, 359 and 509 days.



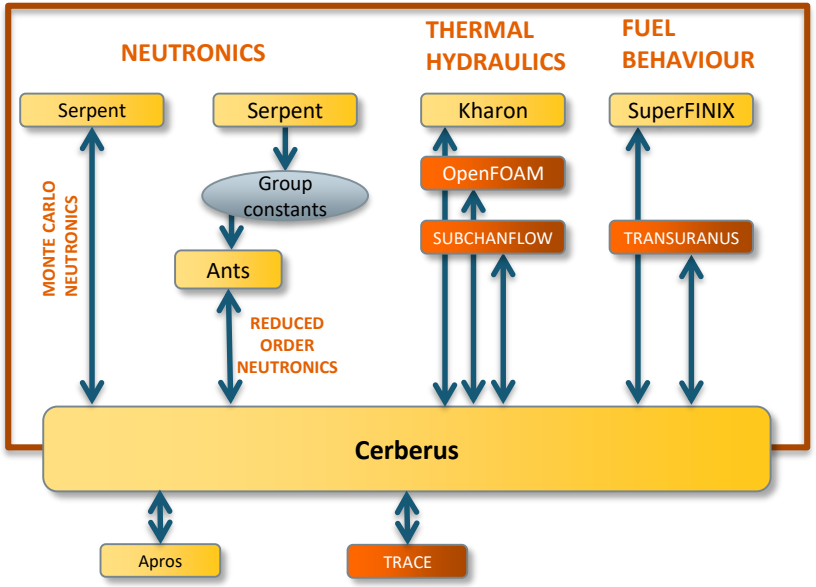
Starting an SMR from hot zero power to full power over several days. Modelled with Ants-SUBCHANFLOW.
Top row: Reactor power and maximum volume averaged fuel temperature during the first hour of the startup
Bottom: Reactor power and concentrations of ^{135}I and ^{135}Xe during the first 40 hours of the startup process.
Dashed lines indicate hot full power steady state values.

Development history and future plans

2022 (ongoing):

Various applications in McSAFER. Validation in LONKERO.

- Coupling to TRANSURANUS via TUWrap, coupling to Apros.
- Ants axial rehomogenization.
- First one-day Kraken training (McSAFER training course).
- First international Kraken workshop at an ANS conference (PHYSOR2022)



Valtavirta, V., Lauranto, U., Rintala, A.
Evaluating the X2 initial core zero power physics tests with Serpent–Ants
PHYSOR 2022, May 15-20, 2022, Pittsburgh, PA

Tuominen, R., Komu, R., Valtavirta, V.
Coupling TRACE with Nodal Neutronics Code Ants Using the Exterior Communications Interface and VTT's Multi-Physics Driver Cerberus
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Leppänen, J., Valtavirta, V., Rintala, A., Hovi, V., Tuominen, R., Peltonen, J., Hirvensalo, M., Dorval, E., Lauranto, U., Komu, R.
Current Status and On-Going Development of VTT's Kraken Core Physics Computational Framework, Energies 15 (2022)

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Verification of Ants time-dependent nodal neutronics model
M.Sc. Thesis, Department of Applied Physics, School of Science, Aalto University.

Valtavirta, V., Rintala, A., Lauranto, U. "Pin power reconstruction for hexagonal geometry in nodal neutronics program Ants"
Submitted to Annals of Nuclear Energy

Current status of Kraken

- Capabilities ready for stationary, operating cycle and transient analyses.
- Modular structure with several options for different solver modules.
- Validation work for safety analyses ongoing (a large future topic).
- Widely used in the core design of VTT‘s district heating reactor concept LDR-50.
- Applied in EU-McSAFER to REA and MSLB analyses of the NuScale concept.

J. Leppänen *et al.* “Load Follow Simulations for the LDR-50 District Heating Reactor Using the Kraken Computational Famework.” PHYSOR2022, Thursday, Core Analysis Methods: III, Haselton 1:30-3:15 PM

J. Leppänen *et al.* “A Finnish district heating reactor: Background and general overview”. Proceedings of ICONE-28, August 4-6, 2021, Virtual Conference, USA.

J. Leppänen *et al.* “A Finnish district heating reactor: Neutronics design and fuel cycle simulations”. Proceedings of ICONE-28, August 4-6, 2021, Virtual Conference, USA.

- REA:
  - Ants – SUBCHANFLOW.
  - Serpent – SUBCHANFLOW.
  - Serpent – SUBCHANFLOW – TRANSURANUS.
- MSLB:
  - Ants – TRACE.
  - Ants – TRACE – OpenFOAM.

Future plans

- Distribution for non-commercial use via OECD/NEA Data Bank and RSICC.
- Development of Ants nodal neutronics program continues:
    - Adjoint flux solver and related capabilities.
    - Improved group constant models.
    - From diffusion to transport?
- Validation for safety analyses:
    - International benchmarks.
    - Finnish NPP models.
- Improved capabilities for reactor design (LDR-50 development).
- Secondary analyses: Final disposal, radiation shielding, dosimetry, safeguards etc.

Licensing and distribution

Licensing and distribution

- Ongoing work for drafting a non-commercial license, establishing export control practices and starting distribution via OECD/NEA Data Bank and RSICC.
- Practices similar to Serpent 2.2.0.
- Initially covers:
  - The **Ants** nodal neutronics code.
  - The **FINIX** fuel performance code.
  - The **SuperFINIX** core level fuel behaviour solver.
  - The **Kharon** thermal hydraulics code.
  - The **libFluid** fluid properties library.
  - The **Cerberus** multi-physics driver package.
  - The **KrakenTools** package of accessory modules.
- Further modules most likely added on yearly basis (requires modifications to licenses and export control documents).
- At this point, changes may still happen between updates.

VTT

beyond
the obvious

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Some references 2018 - 2019

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