# Kraken workshop

## Introduction to the Kraken framework

Ville Valtavirta

21/04/2024 VTT – beyond the obvious

# Outline

- What is Kraken?

- Coupling scheme in Kraken
- Physics solvers involved

- Current status
- Future plans
- Licensing and distribution

- Getting started

# What is 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.

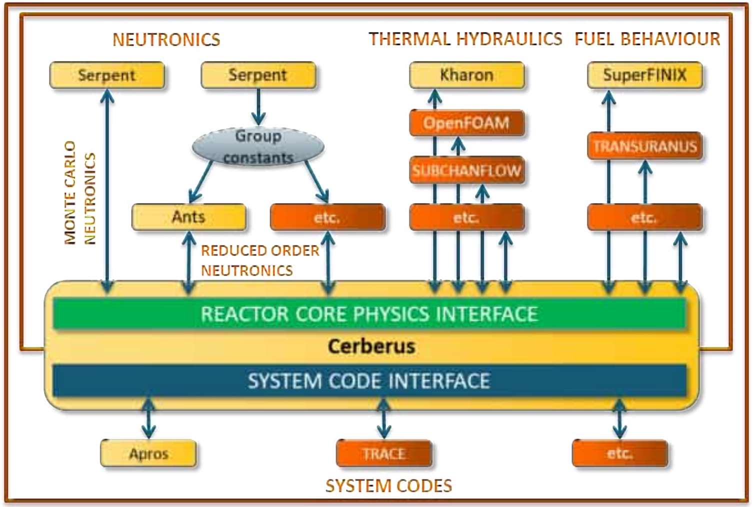
Kraken provides VTT with the **tools** required for future safety analyses and the **expertise** to use those tools in a proper manner.

Kraken is designed both for **independent deterministic safety analyses**, **evaluation of new reactor concepts** and as a **general research tool**.

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.

**International distribution** for **non-commercial use** through OECD/NEA Data Bank and RSICC (Spring 2024).




A schematic representation of the 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.

# Code coupling approach in Kraken

# Couplings for coupled calculations

**A central multi-physics driver Cerberus:**

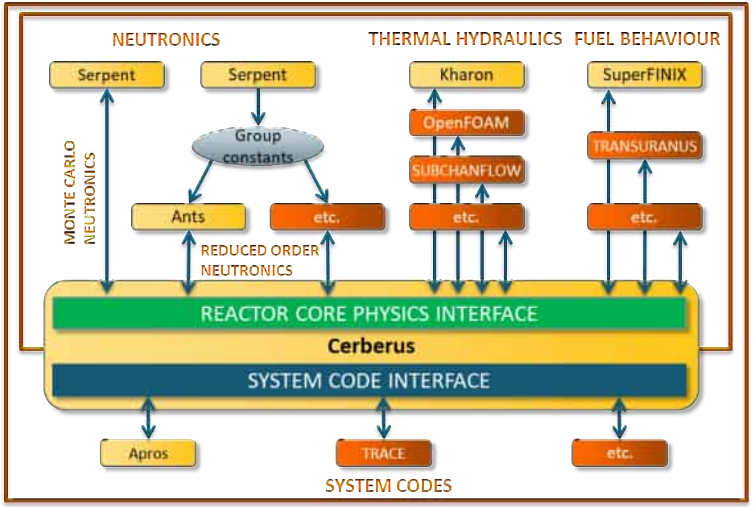
- Each solver only needs to communicate with Cerberus.

**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.
- Easy to couple new solvers.
  - See https://serpent.vtt.fi/kraken/index.php/Code_coupling_in_Kraken

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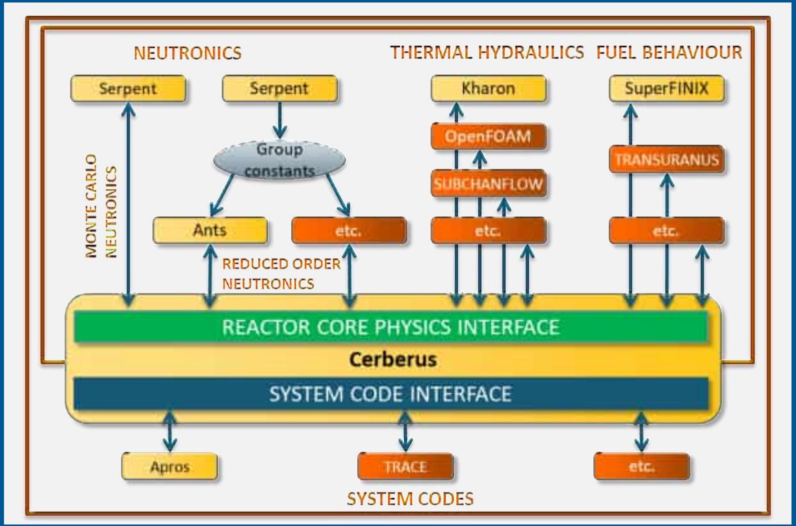
# Physics solvers

# Physics solvers related to Kraken

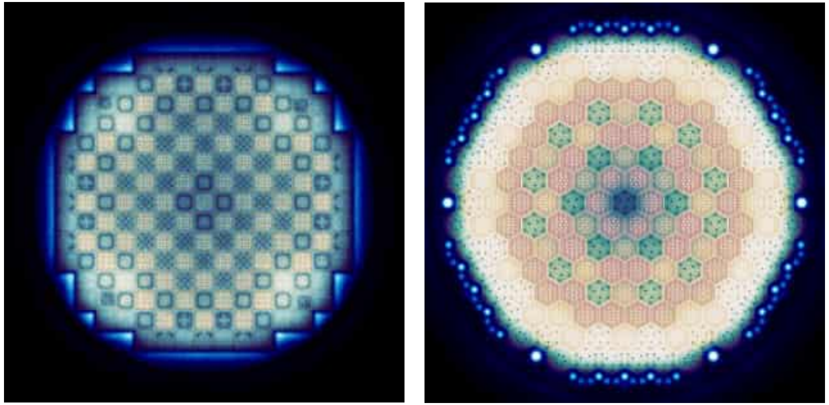
- **Neutronics solvers**
  - **Serpent – available for non-commercial/commercial use.**
  - **Ants – available as part of Kraken 1.2.**
- **Thermal hydraulics solvers**
  - **Kharon – available as part of Kraken 1.2.**
  - OpenFOAM – publicly available.
  - SUBCHANFLOW – owned by KIT.
- **Fuel behavior solvers**
  - **FINIX – available as part of Kraken 1.2.**
  - **SuperFINIX – available as part of Kraken 1.2.**
  - TRANSURANUS – owned by JRC.
- **System codes**
  - Apros – commercial product of Fortum and VTT.
  - TRACE – owned by NRC.

# Neutronics


NEUTRONICS
THERMAL HYDRAULICS
FUEL BEHAVIOUR
Serpent
Serpent
Kharon
SuperFINIX
Group constants
OpenFOAM
TRANSURANUS
SUBCHANFLOW
MONTE CARLO NEUTRONICS
Ants
etc.
etc.
etc.
REDUCED ORDER NEUTRONICS
REACTOR CORE PHYSICS INTERFACE
Cerberus
SYSTEM CODE INTERFACE
Apros
TRACE
etc.
SYSTEM CODES

# Serpent Monte Carlo code

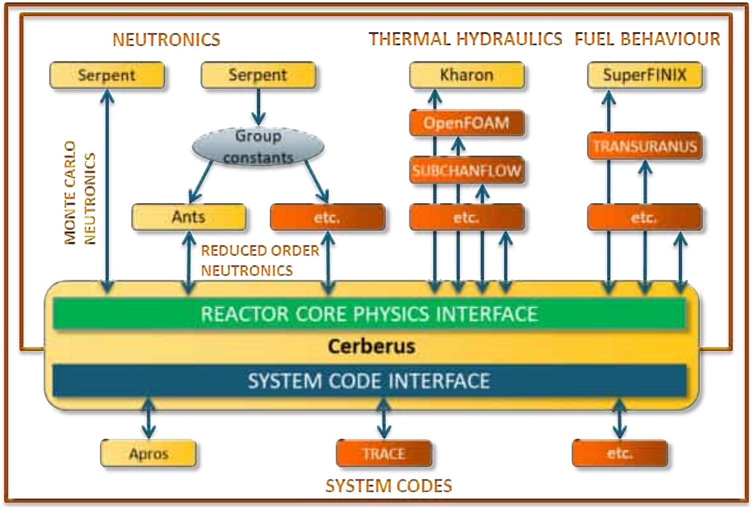
- Continuous-energy Monte Carlo transport calculation code developed at VTT since 2004.
- Neutron, photon and coupled neutron / photon transport modes.
- Originally developed for reactor physics, but scope of applications not limited to reactor modelling
- Advanced features and capabilities:
  - Automated procedures for burnup calculation and group constant generation
  - Multi-physics interface for thermal hydraulics and fuel performance code coupling
  - Domain decomposition enabling core-level burnup calculations
  - Transient simulation mode with delayed neutron physics
  - Methods for sensitivity and uncertainty analysis
  - Support for CAD- and unstructured mesh-based geometries
  - Weight-window based variance reduction techniques with built-in importance solver
  - ...



Serpent meshplots for BEAVRS (left) and Khmelnitsky 2 (right) initial core. Warm colors indicate fission power and cold colors indicate thermal flux.

# Serpent Monte Carlo code

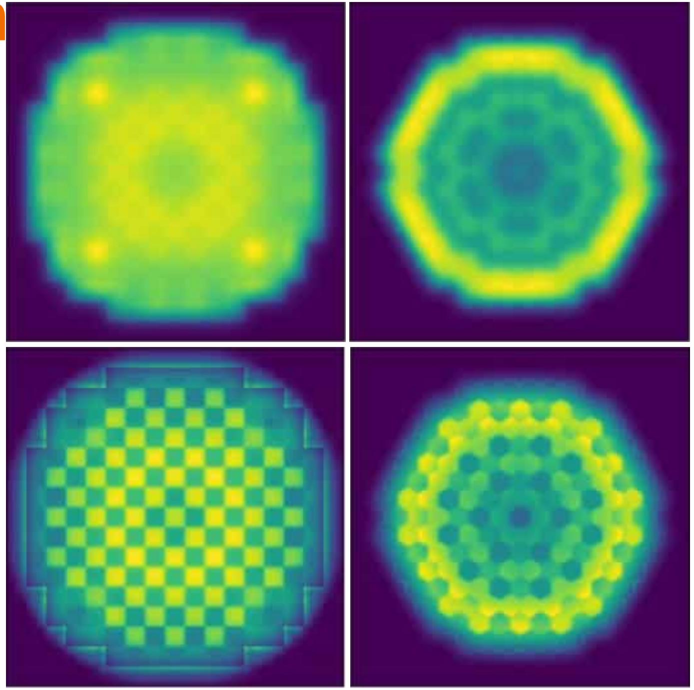
- Dual role in the Kraken framework:
  1) Group constant generation for the Ants nodal neutronics code (reduced-order sequence)
  2) Direct coupling to other physics solvers (high-fidelity sequence)
- The Serpent-based high-fidelity sequence can be used for best-estimate analyses or verification of reduced-order calculations without major modifications in the configuration
- New base version 2.2.0 released in May 2022, three licensing options:
  - Single-user licenses from OECD/NEA Data Bank and RSICC – free of charge for non-commercial research and educational use
  - Commercial license – agreement with VTT, license fees applied
  - Reduced academic license for unlimited number of users (“professor license”) – agreement with VTT, one-time processing fee applied
- Serpent has currently more than 1000 users in 250 organizations in 44 countries around the world




Serpent serves a dual role in the Kraken framework.

# Ants nodal neutronics program

- Multi-group nodal neutronics code developed at VTT since 2017.
- Single program for all nodal neutronics calculations at VTT
  - Excluding Apros nodal models.
  - Previously multiple programs:
    - In-house: HEXBU-3D, TRAB-3D, HEXTRAN.
    - Third-party: SIMULATE3.
  - Many features beyond their capabilities, some lagging behind due to development resources and focus.
- Currently solves the nodal diffusion equation.
- Flux solution methodology based on combination of AFEN and FENM nodal methods.
- Rectangular, hexagonal and triangular nodal geometries supported.
  - Triangular geometry supported only for hexagonal assembly lattice.
  - Axial mesh refinement for all geometries, radial refinement for rectangular and triangular geometry.



Ants fast (top) and thermal (bottom) homogeneous flux distributions for BEAVRS (left) and Khmelnitsky 2 (right) initial core.

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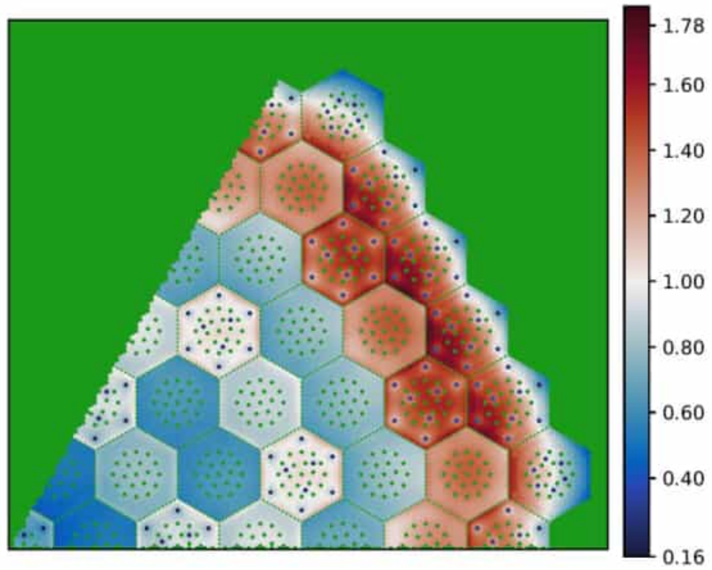
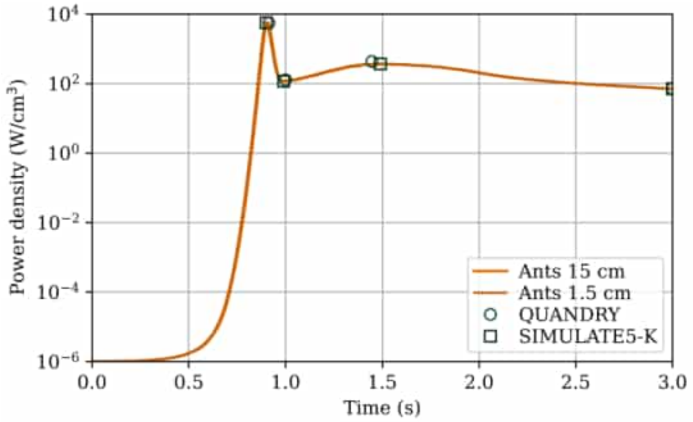



Ants evaluation of the relative pin power distribution in one sextant of the X2 benchmark core.

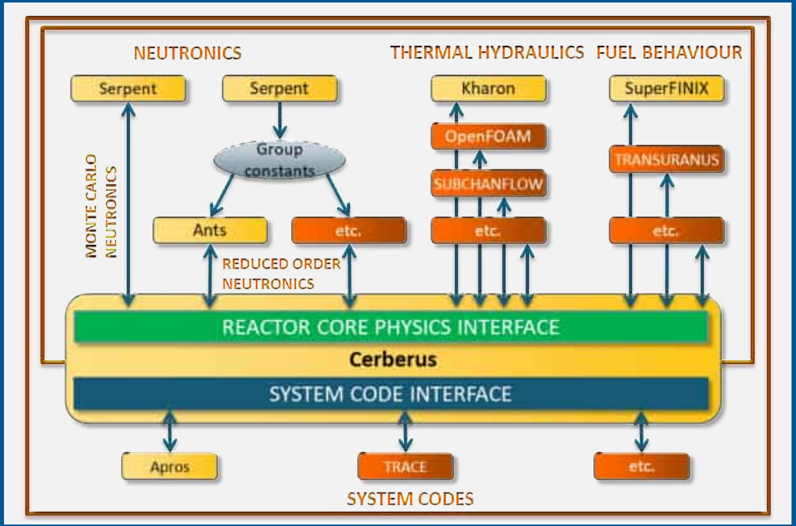
# Ants nodal neutronics program

- Steady state, burnup and transient calculation methodologies with support for external fixed source.
- Steady state solved for critical k-eigenvalue or boron concentration, or with external fixed source.
- Supports e.g. pin power reconstruction (support for triangular geometry not yet implemented), predictor-corrector methods in depletion, microscopic depletion (e.g. inventory calculations) with CRAM.
- Ants serves as the reduced order neutronics solver in Kraken providing solutions to stationary, depletion and transient neutronics problems with reasonable computational time.
- Development and validation work ongoing.




Time-dependent powers of Ants and other nodal programs in the LRA single rod benchmark transient.

# Thermal hydraulics



# Kharon thermal hydraulics solver

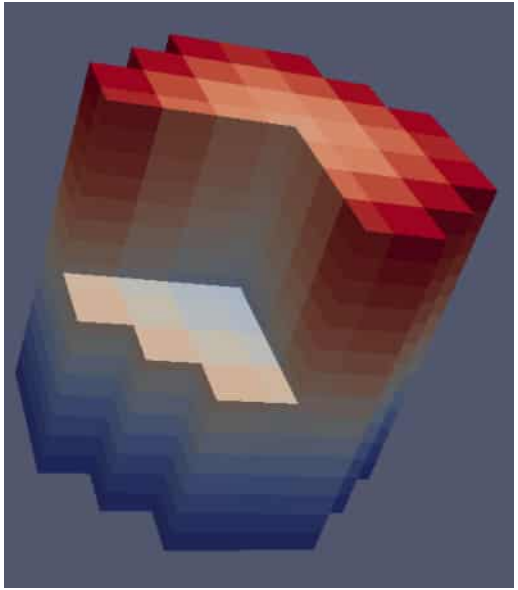
A simple core level thermal hydraulics solver developed at VTT:

- Two phase.
- Time-independent.
- Closed channel.
- Porous medium.

Models flow based on channel inlet and outlet boundary conditions and basic geometry.

Also models heat transfer from fuel rod cladding to coolant providing boundary condition for fuel behaviour codes.

Utilized in stationary and fuel cycle simulations. Transient simulations need another tool.



# OpenFOAM for computational fluid dynamics

Open source software for CFD modelling and other purposes: [https://openfoam.org/](https://openfoam.org/)

VTT is a contributor in the project.

Past history in coupling Serpent and OpenFOAM in many ways.

Kraken applications have used a porous medium approach with a modular solver based on the multiPhaseEuler solver.

Applications with Kraken:

- Stationary and transient coarse mesh solutions inside the reactor core.
- Mixing, natural circulation etc. inside the reactor pressure vessel.

# SUBCHANFLOW thermal hydraulics solver

Subchannel level TH-solver developed by KIT.

https://www.inr.kit.edu/english/1008.php

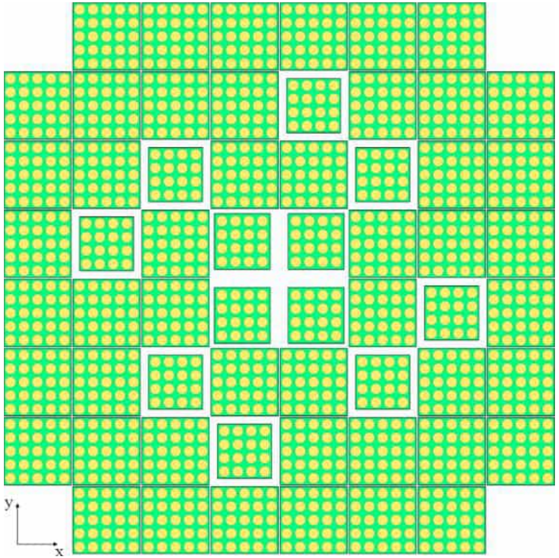
Long history in coupling Serpent and SUBCHANFLOW using various approaches.

Most recently in the McSAFE and McSAFER projects,

Kraken coupling utilizes the pre-existing C API and a Kraken-specific wrapper layer (SCFWrap) to handle communications to/from Cerberus.

Applied in stationary, depletion and transient analyses.

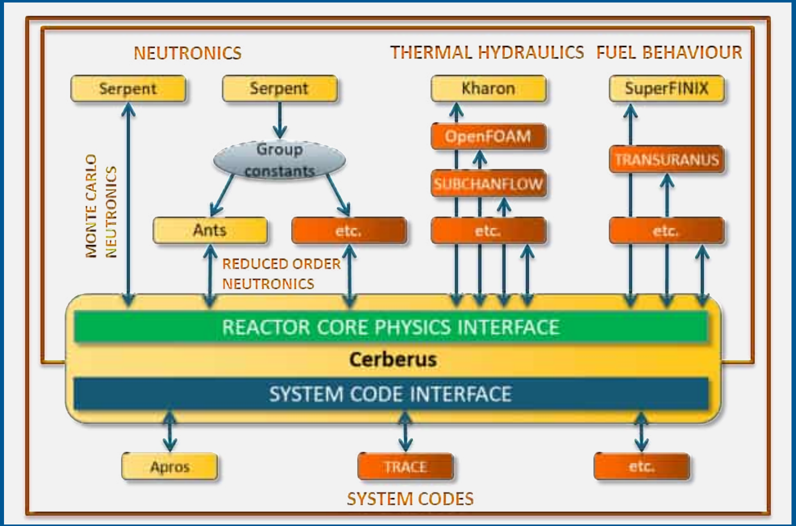
Python preprocessor created in McSAFE utilized in generation of calculation mesh and interpolations.




Plot of the SCF model for the SPERT-IIIE core.

D. Ferraro *et al.*, "Serpent/SUBCHANFLOW pin-by-pin coupled transient calculations for the SPERT-IIIE hot full power tests", Annals of Nuclear Energy 142 (2020)

# Fuel behaviour



# FINIX fuel behaviour module

The FINIX fuel behaviour module has been developed at VTT since 2012.

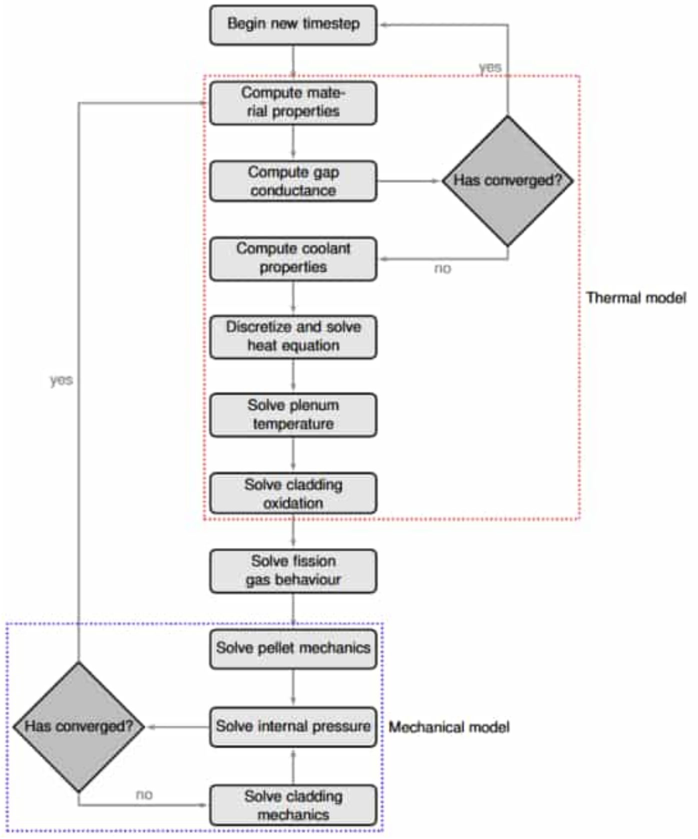
FINIX is a traditional 1.5-dimensional single rod fuel performance code.

Originally developed as a simple fuel behaviour solver module that could be coupled to reactor analysis codes at the source code level.

Developed for LWR applications.

Verified against FRAPTRAN and FRAPCON in RIA and steady state scenarios and compared against experimental Halden reactor data.

In the Kraken framework, FINIX is used through SuperFINIX, the core level fuel behaviour solver.




Overview of the FINIX solution model.

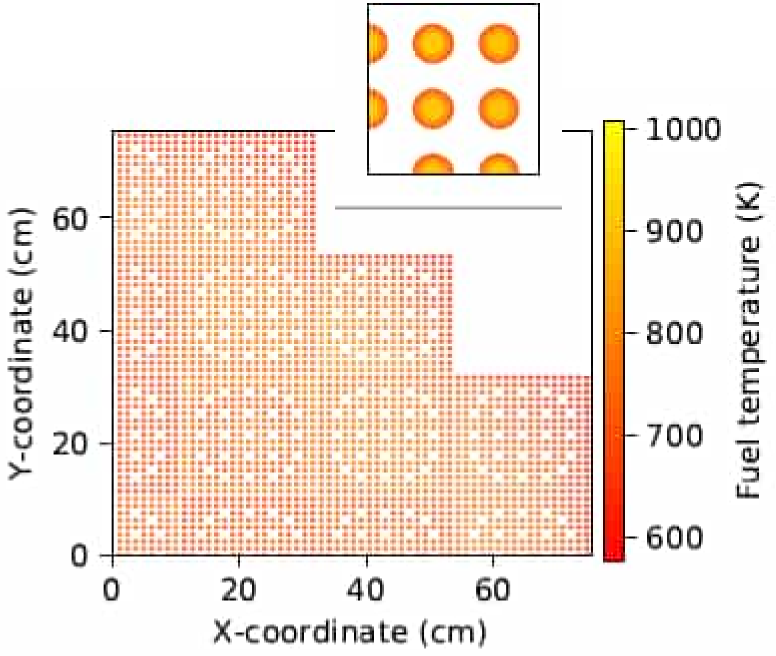
# SuperFINIX core level fuel behaviour solver

The SuperFINIX core level fuel behaviour solver was written in 2019.

FINIX models a single fuel rod. LWR cores contain hundreds of fuel assemblies, tens of thousands of fuel rods.

Flexible fidelity for field input and output:

- Nodal codes, such as Ants require one fuel temperature value per node.
- Monte Carlo codes, such as Serpent can utilize individual rod radial distributions for fuel temperatures.
- Conversely power distribution may be evaluated at assembly, quarter assembly, rod or sub-rod level.
- SuperFINIX accepts input fields and provides output fields at multiple levels of discretization for the same model.




High fidelity fuel temperature fields taken from SuperFINIX.

# TRANSURANUS fuel performance code

European fuel performance code developed by the JRC.

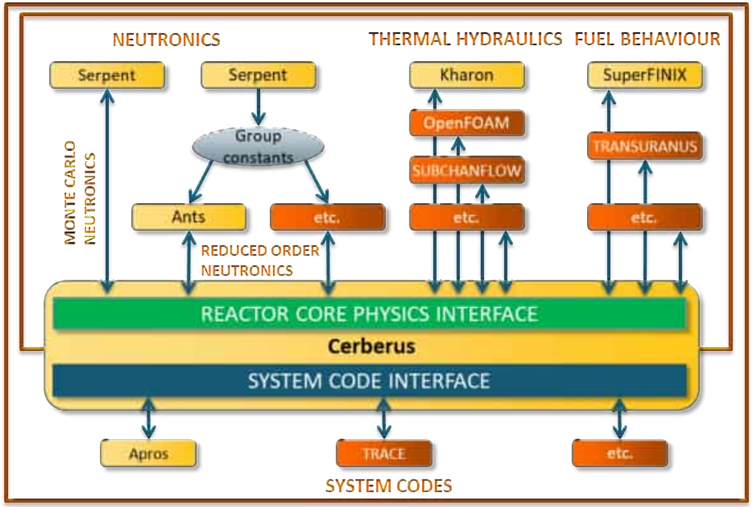
https://data.jrc.ec.europa.eu/collection/transuranus

Coupled with Serpent in the McSAFE project.

Single rod solver, but Kraken coupling utilizes pre-existing C and C++ layers and a Kraken-specific wrapper layer (TUWrap) to handle communications to/from Cerberus and to handle the core level solution.

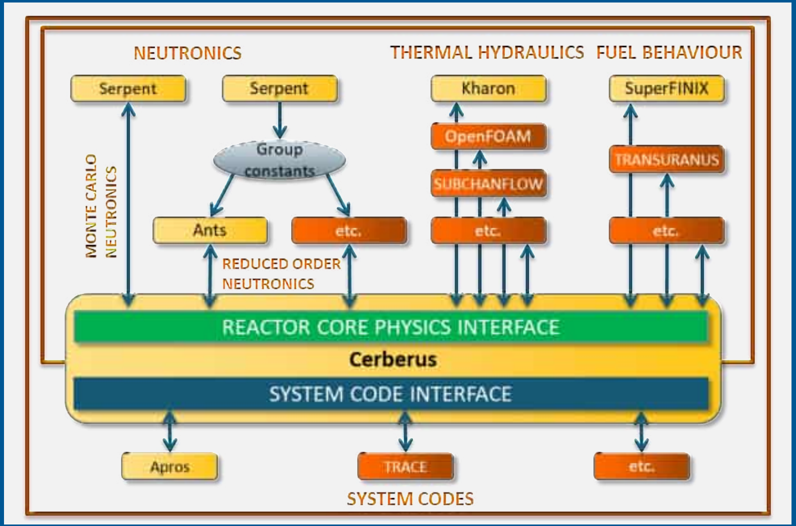
To be applied in stationary, depletion and transient analyses.

Python preprocessor created in McSAFE utilized in generation of calculation mesh and interpolations.




TRANSURANUS is one of the possible fuel performance codes that can be used with Kraken.

# System codes



# Apros

A system code / process simulator developed at VTT and Fortum for a long time.

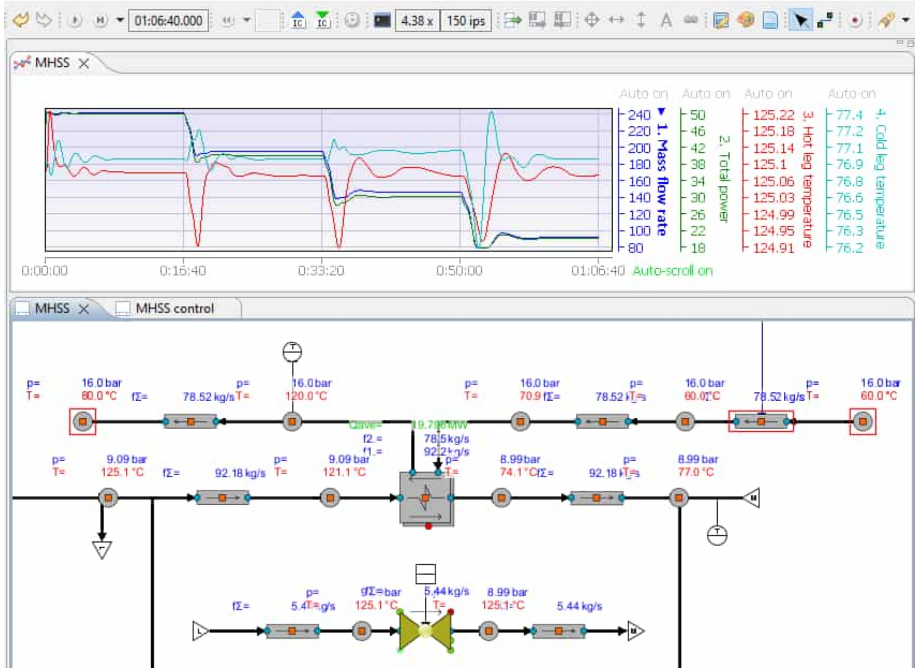
https://www.apros.fi/

Used in the safety analyses of Finnish NPPs.

Also used extensively in VTT's development work of the LDR-50 district heating reactor concept.

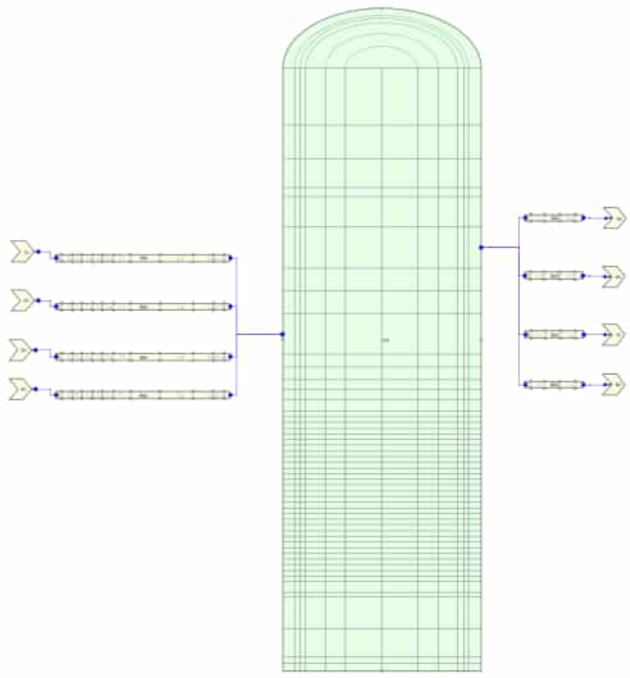
Basic coupling with Kraken achieved allowing the use of Ants as a 3D core nodal solver for Apros simulations.

E. Silvennoinen et al., "The APROS software for process simulation and model development", Technical Research Centre of Finland, Research reports 618 (1989).



# TRACE

- TRAC/RELAP Advanced Computational Engine (TRACE)
- A system code developed by US NRC for LWR transient analyses.
- Being adopted in Finland for independent deterministic safety analyses.
- Finland participates in US NRC's Code Applications and Maintenance Program (CAMP).
- Coupled to Kraken using a separate wrapper TRACEWrap*, which communicates with TRACE using the Exterior Communications Interface (ECI).
- Used as an independent verification tool for Apros analyses in Finland.

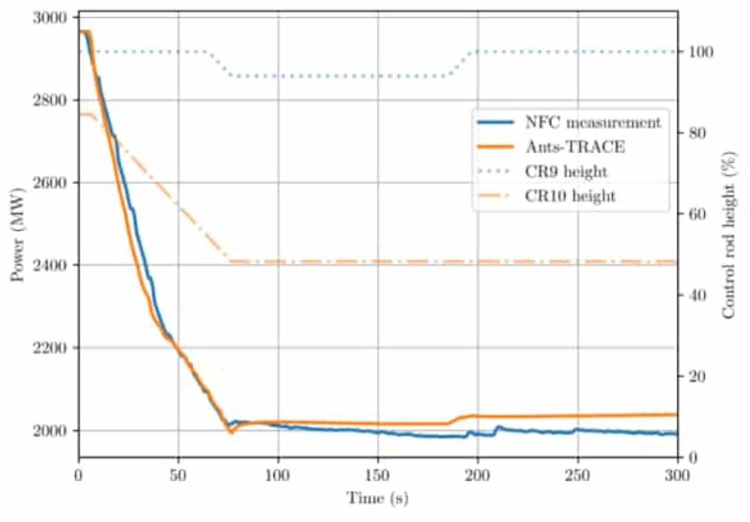


*Tuominen, R., Komu, R., Valtavirta, V.,
Coupling TRACE with Nodal Neutronics Code Ants Using the Exterior Communications Interface and VTT's Multiphysics Driver Cerberus
PHYSOR 2022, May 15-20, 2022, Pittsburgh, PA

# Recent and near future applications

# Recent applications

- **VVER-1000 transient modelling.**
- SMR transient modelling (McSAFER).
- SMR fuel cycle simulations (LONKERO, EASI-SMR).
- SMR core design (LDR-50).
- Full core inventory calculations (NOTCO).
- VVER-1000 fuel cycle simulations (X2 validation).
- VVER-440 fuel cycle simulations (EVEREST).
- PWR fuel cycle simulations (EVEREST).
- High-fidelity research reactor modelling (EVEREST).
- Pebble bed reactor modelling.




Reactor power in the Kalinin 3 main circulation pump trip scenario.

Lauranto, U., Komu, R., Rintala, A. and Valtavirta, V.
"Validation of the Ants-TRACE code system with
VVER-1000 coolant transient benchmarks." Ann. Nucl. Energy, 190 (2023) 109879.

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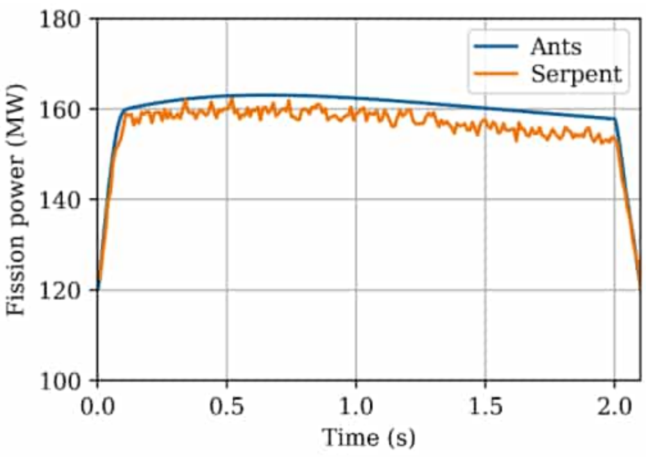


Total reactor power in the NuScale-like REA scenario. Ants-SUBCHANFLOW vs. Serpent-SUBCHANFLOW-TRANSURANUS.

McSAFER project WP3.

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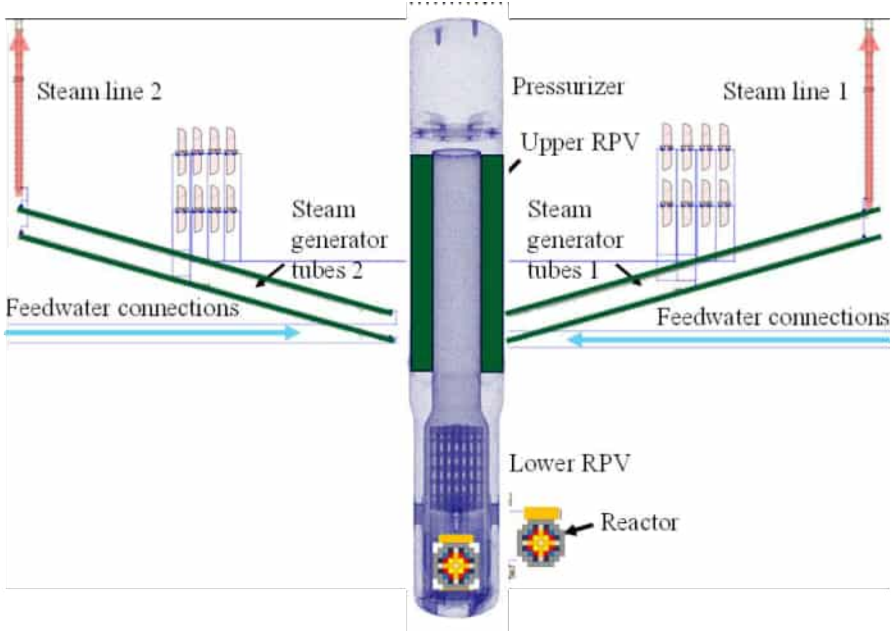


Schematic representation of the TRACE-Ants-OpenFOAM coupling applied to the NuScale-like MSLB scenario.

McSAFER project WP5.

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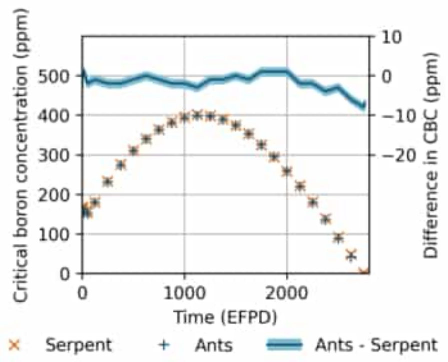


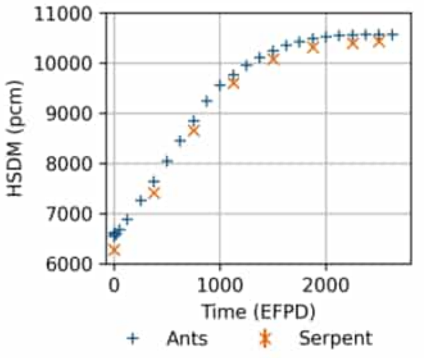


Critical boron concentration during one cycle of an SMR operation and the hot shutdown margin evaluated by Ants-Kharon-SuperFINIX and Serpent-Kharon-SuperFINIX.

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

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[REDACTED]

See https://www.ldr-reactor.fi/en/1099-2/
and presentation by Jaakko Leppänen.

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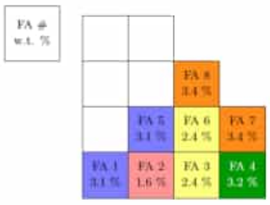


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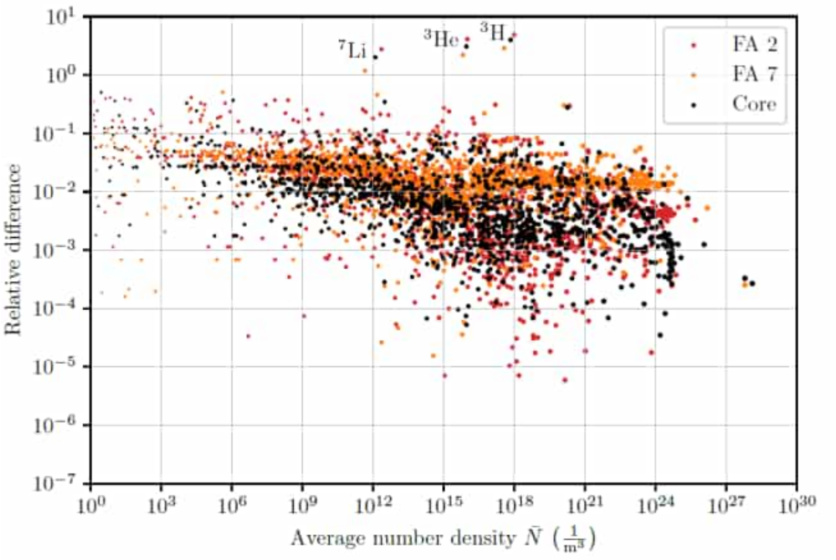


The average number density of each nuclide calculated with Ants and their relative difference compared to Serpent in the 3D SMR core depletion problem. The size of the data point is proportional to the logarithm of the nuclide number density. Three outliers at the top of the figure are labeled with their names.

Kähkönen, T.
“Calculating spent nuclear fuel composition for secondary nuclear safety analyses using nodal diffusion neutronics.”
M.Sc. Thesis, Department of Applied Physics, School of Science, Aalto University, 2022.

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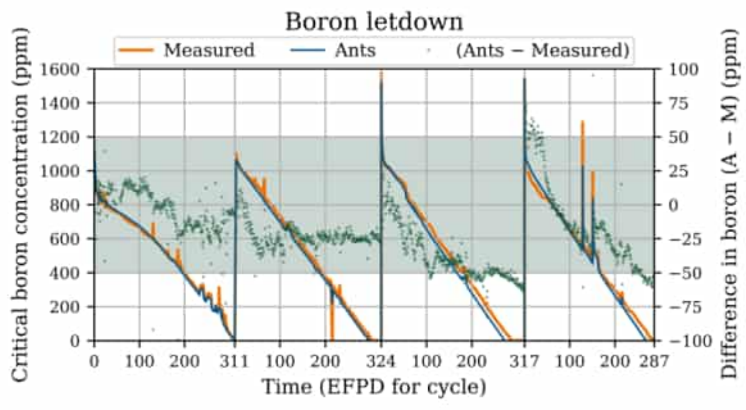
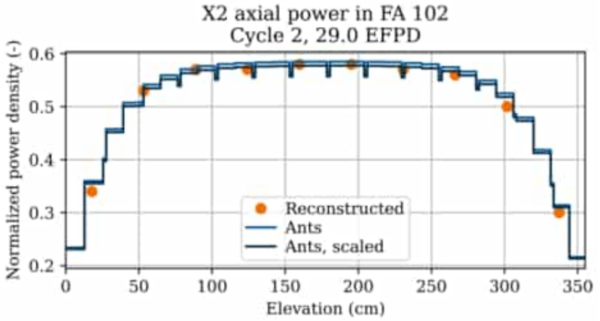



Measured and calculated boron letdown curves over the first four cycles of the Khmelnitsky NPP unit 2.




Measured/reconstructed axial power distribution in assembly 102 at 29 EFPD of cycle 2 of Khmelnitsky NPP unit 2 and Kraken prediction.



Valtavirta, V. and Rintala A.
"Validating Kraken for VVER-1000 fuel cycle simulations using the X2 benchmark." Ann. Nucl. Energy, 190 (2023) 109878

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Starting in 2024. Modelling of fuel cycles for Paks NPP in European project EVEREST.

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Starting in 2024. Modelling of fuel cycles for Grohnde NPP (pre-Konvoi) in European project EVEREST.

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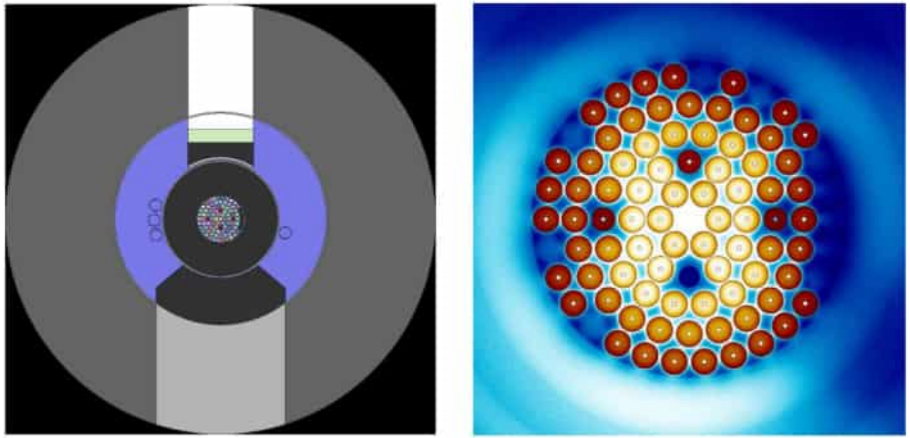
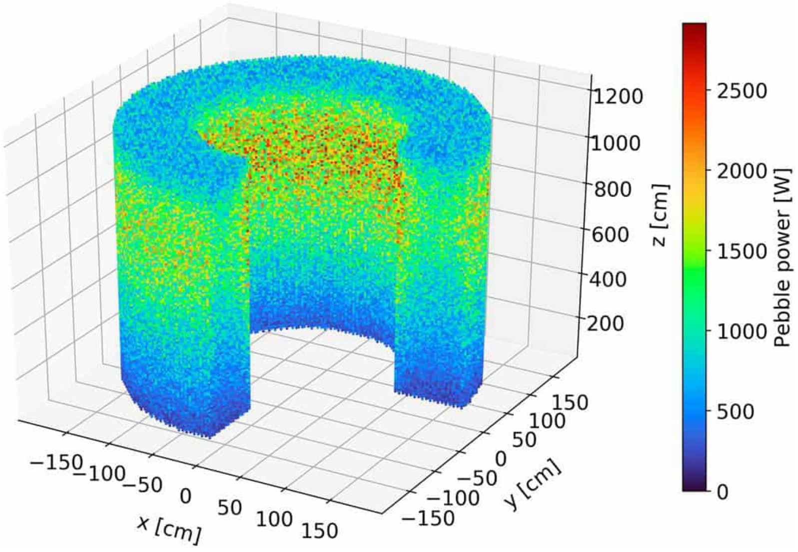
- Pebble bed reactor modelling.



Serpent model geometry plot and meshplot of the reactor core of the JSI TRIGA. Starting in 2024, modelling of the TRIGA in high fidelity with Serpent and OpenFOAM.

# Recent applications

- VVER-1000 transient modelling.
- SMR transient modelling (McSAFER).
- SMR fuel cycle simulations (LONKERO, EASI-SMR).
- SMR core design (LDR-50).
- Full core inventory calculations (NOTCO).
- VVER-1000 fuel cycle simulations (X2 validation).
- VVER-440 fuel cycle simulations (EVEREST).
- PWR fuel cycle simulations (EVEREST).
- High-fidelity research reactor modelling (EVEREST).
- **Pebble bed reactor modelling.**




Pebble power distribution at a representative equilibrium conditions.


Robert, Y., Siaraferas, T. and Fratoni, M.
“Hyper-fidelity depletion with discrete motion for pebble bed reactors.” Sci Rep 13, 12711 (2023).
https://doi.org/10.1038/s41598-023-39186-3

# Future plans

# Future plans for Kraken

- Distribution for non-commercial use via OECD/NEA Data Bank and RSICC.
  - OECD/NEA Data Bank: https://www.oecd-nea.org/tools/abstract/detail/nea-1924
  - RSICC: To be announced.
- Development of Ants nodal neutronics program continues.
  - Treatment of axial discontinuities.
  - Improved group constant model or group constant models for different applications.
  - From diffusion to transport (SP3).
- HTGR applications?
- Wider range of Serpent applications through Kraken.
  - Spent fuel secondary analyses (final disposal, radiation shielding)?
  - Dosimetry?
  - Fusion neutronics?
- Validation for safety analyses:
  - International benchmarks and Finnish NPP models.
- Improved capabilities for reactor design (with LDR-50 development).
- Educational use.
- Usability, input and output improvements.

# Licensing and distribution

# Licensing and distribution

- 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 Python package.
  - The **KrakenTools** Python package of accessory modules.
  - The **Cetus** reactor core simulator Python package.
- Further modules may be added when needed.
- At this point, (breaking) changes are still likely to happen between updates.

# Disclaimer and getting started

# Disclaimer and getting started

Kraken is developed at VTT largely for VTT's own reactor analysis needs and is provided for non-commercial research and education use, free of charge, with no guarantees that it will be applicable to your specific modelling problem. Please verify and validate the calculation chains for your specific application before trusting the results.

At the distribution of Kraken 1.2 we consider Kraken to be in an “early access” phase, where some parts of the framework are in a well functioning state and provide good results for specific applications, but other parts are still severely lacking. The documentation is not complete, and the installation can be a challenge. You can report any problems you encounter to us at the Kraken forum. We will be happy to get this feedback, but likely are not able to resolve the problem for you.

During version updates, we try to not break the existing inputs, but cannot guarantee full backwards compatibility at this early stage of development.

All that said, we hope you find some use in this framework and are also happy to hear about any successful modeling achievements (not only problems)!

# Disclaimer and getting started

Get Kraken from:

- OECD/NEA Data Bank: https://www.oecd-nea.org/tools/abstract/detail/nea-1924
- RSICC: <in future>

Check the Kraken Wiki for installation instructions and tutorials (including these slides):
https://serpent.vtt.fi/kraken/index.php/Main_Page

Documentation in Kraken Wiki will be continuously updated (within available resources).

Check the Kraken forum for the most recent discussion by users:
https://ttuki.vtt.fi/serpent/viewforum.php?f=10

# beyond
## the obvious

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