MULTI-PHYSICS COUPLING FOR NUCLEAR SYSTEMS

(Les couplages multi-physiques)

Réunion plénière du Conseil Scientifique (CS) de l'IN2P3

"La physique nucléaire pour l'énergie"

Jeudi 3 Février 2022

N. Capellan, V. Ghetta, J. Giraud, P. Rubiolo

Outline

- Why Developing Multi-physics Models for Nuclear Reactors?
- State of Art, Scientific Challenges and Motivation
- Overview of the Numerical and EXperimental MUltiphysicS Program (NEXUS)
- Numerical Activities
- Perspectives

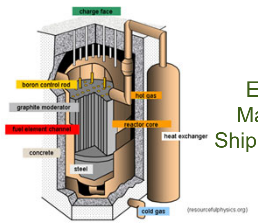
Why Developing Multiphysics Models for Nuclear Reactors?

Reactor Design and Modeling Trends

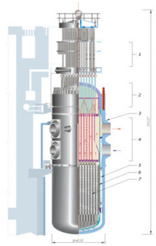
Nuclear Reactor Design Generations

1950 1960 1970 1980 1990 2000 2010 2020 2030

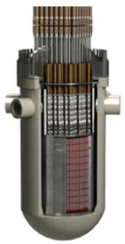
1er Generation | 2nd Generation | 3rd Generation | 3^{+} Generation | 4th Generation



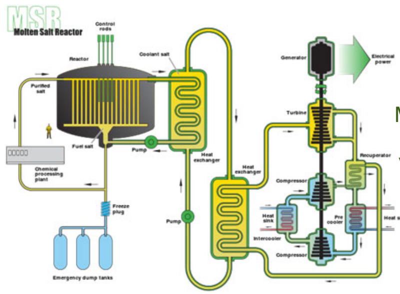
EBR-I, Magnox, Shippingport, etc



PWR, BWR, Candu, VVER, etc.



AP600, AP1000, EPR, ABWR, etc.

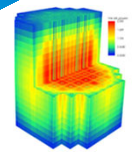


MSFR, SFR, VHTR

Methods and Tools used for Reactor Design and Safety Studies

1950 1960 1970 1980 1990 2000 2010 2020 2030

- 1950: Semi-empirical correlations + Experiments
- 1970: Semi-empirical correlations + 0D/1D models standalone
- 1990: 2D/3D semi-empirical standalone models + PIE/operation feedback from reactor fleet
- 2000: 3D models with coupling + CFD - Monte Carlo
- 2020: Multi-physics and multi-scale coupled models for design and safety + BE Plus Uncertainties (BEPU)

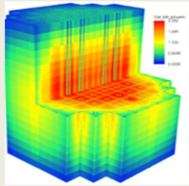


"Full core numerical model"

What is a Multiphysics model?

- A multi-physics numerical model usually refers today to an algorithm that numerically solves a set of coupled equations

  - **Equations which represent physical laws** describing a set of phenomena taking place in the nuclear system:
    - Mass, momentum and energy conservation,
    - Neutron (or gamma-ray) transport,
    - Nuclear and chemical reactions, etc.



  - **Equations usually developed from first principles** and thus models should involve very few assumptions. All relevant phenomena are considered (PIRT).
  - **Equations are (more or less simultaneously) solved** with the couplings between phenomena. Some couplings could be multiscale.
  - **Equations in Multiphysics models usually provide high fidelity results** both concerning the space (3D when a flow is involved) and time scales

- The results are often considered as Best Estimates (BE) values

Advantages and Drawbacks

Advantages

- Provide results with higher accuracy than previous codes that can be considered as Best Estimates (BEs) values
- Access to information at space and time scales not previously possible from experiments/models
- Allow to study the effects of individual couplings
- Better estimation of the design and safety margins: enabling potential gains of margins

Drawbacks and Challenges

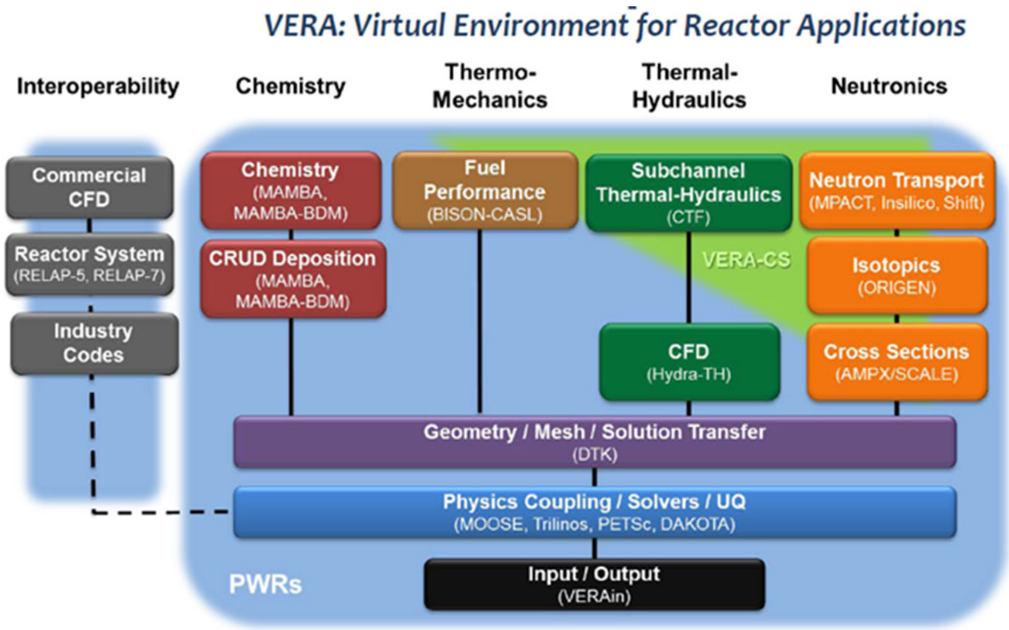
- Must include all the relevant phenomena and the associated interactions (need a PIRT)
- Require very high computation resources
- Large amounts of input data have to be fed to these models (properties, geometry, IC, BC, etc.)
- Achieving adequate stability, convergence and consistency is not straightforward
- They require novel safety methodologies involving uncertainty propagation
- Licensing of these methods and tools for reactor safety studies is very challenging

State of Art, Scientific Challenges and Motivation

State of Art: The VERA Platform Example

- Several ongoing initiatives worldwide for developing and sharing multiphysics models for nuclear reactors

- In the USA, the CASL consortium has developed the VERA platform since 2010:
  - One of the most complete multiphysics platform for reactors
  - Models most of the phenomena of interest for Pressurized Water Reactors (PWRs)
  - Uses operator splitting strategy
  - Developed from existing commercial and academic codes
  - Implementation of VERA for safety studies poses significant challenges for safety studies



Source: The Consortium for Advanced Simulation of Light Water Reactors (CASL)
(https://www.ornl.gov/onramp/casl-vera)

Scientific Challenges

- ## Numerical aspects
  - Operator splitting strategy versus tightly coupled schema
  - Surrogate models: Artificial Neural Networks, Polynomial Regressions, Reduce Order Models (ROM), etc.

- ## Phenomena and couplings modeling
  - Some examples: Coupled thermo-mechanics, thermal-hydraulics and neutronics calculations, Transient neutronics simulations based on Monte Carlo codes, Neutronics noise & flow-induced vibrations, Reactor fluid-structure interactions, PWR chemistry studies, Criticality accidents, liquid fueled reactors (MSRs), etc.

- ## Nuclear systems design
  - High fidelity simulation of complex systems (MSRs, MMRs, Space Reactors, Criticality accidents, etc.)
  - Resolution of inverse problems
  - Model-constrained optimization

- ## Nuclear safety methods
  - Development of novel safety methodologies such as BEPU methods: Best Estimate (BE) values provided by multiphysics codes require the determination of the confidence bounds based on an uncertainty quantification methodology
  - Characterization of uncertainties sources: system properties, boundary and initial conditions, physical models, numerical methods, User, etc.
  - Experimental validation (e.g. integral experiments) and numerical benchmarks

Motivation and Interest

- The IN2P3/CNRS has made important contributions to the research on advanced nuclear systems (ADS, MSRs, fuel cycles, etc.)
- The study of advanced nuclear systems will increasingly involve high fidelity simulations based on first principles multiphysics models

- Continue to develop competitive research in the domain of the reactor physics will require to maintain the capability for developing and performing multiphysics numerical simulations for nuclear systems
- Already available at the IN2P3/CNRS: Technical competences and resources (Neutronics, thermal-hydraulics, thermal-mechanics, etc.) for developing meaningful experimental and modeling research on multiphysics for nuclear systems

Overview of the Numerical and Experimental Multiphysics Program (NEXUS)

Goals and Development Strategy

- Goal

"Development of the numerical models and the related multiphysics experiments necessary for advanced nuclear systems where strong phenomena couplings exist"

- Non-goal:

Development of a multiphysics platform for all nuclear systems (PWRs, SFRs, etc.)

- The starting point
  - First coordinated numerical and experimental efforts for multiphysics studies of nuclear systems started in 2015 in the framework of the SAMOFAR project
  - Molten Salt Reactors (MSRs) = excellent nuclear system for multiphysics studies
  - Studies were later expanded to include criticality accidents, targets and space reactors

- The strategy
  - Multiphysics studies focused on small nuclear systems with strong couplings
  - Improve the understanding of the phenomena and the couplings
  - Develop models and experiments all together when it is possible
  - Explore new nuclear design/safety applications of the multiphysics models
  - Develop collaborations with partners and contribute to education and training

Numerical Tools (1/4)

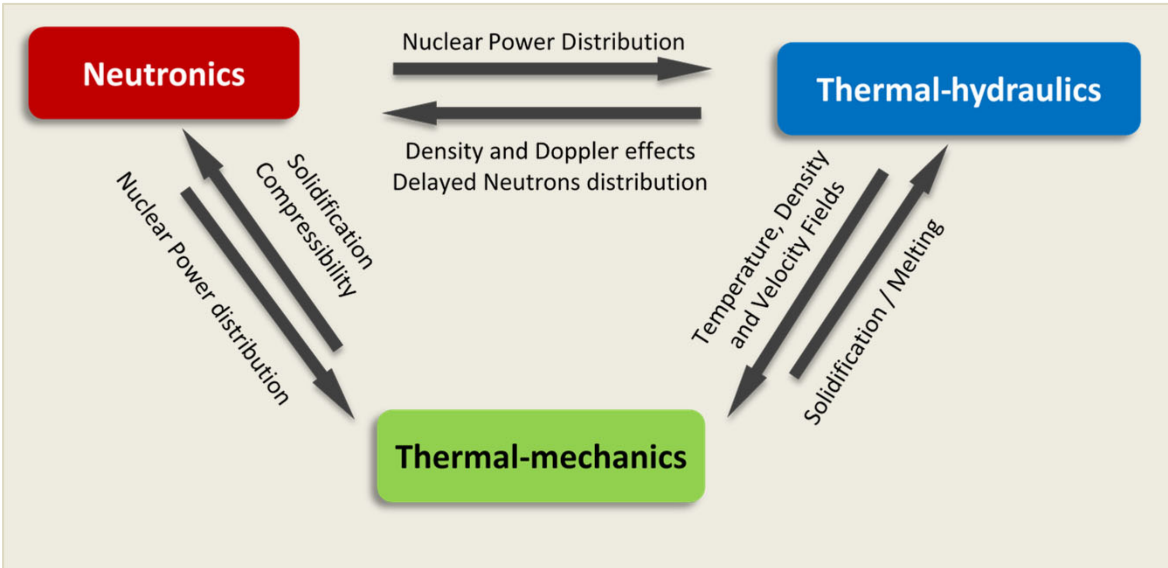
- Initial multiphysics modeling efforts were focalized on the MSFR

- A multi-physics numerical tool was developed based on the numerical coupling between:
  - **OpenFOAM**: C++ toolbox for development of numerical solvers for continuum mechanics problems using Finite Volume Method (FVM), including Computational Fluid Dynamics (CFD)
  - **SERPENT**: multi-purpose 3D continuous-energy Monte Carlo particle transport code

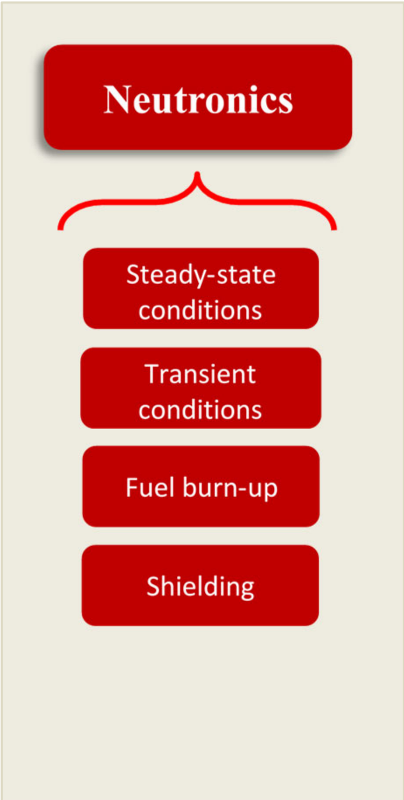
- Different regions can be modeled with the tool: solid and fluid regions

- Three domains:
  - Neutronics
  - Thermal–hydraulics
  - Thermal–Mechanics

- Other tools used in the analyses: ANSYS, SMURE, MCNP, etc.

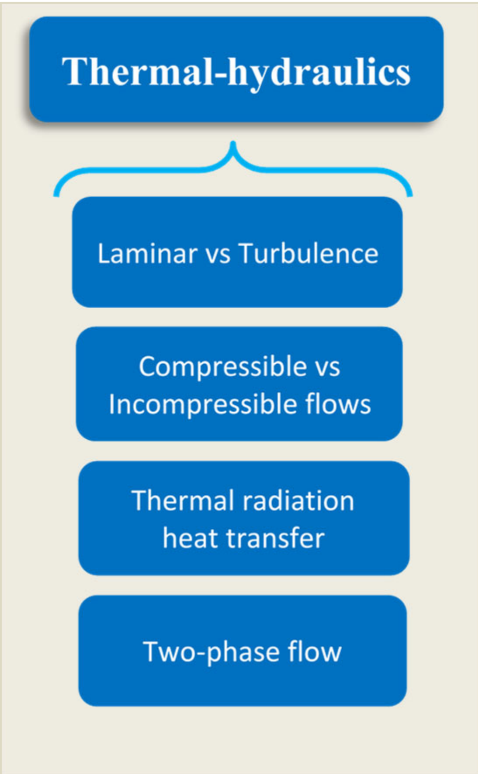


Numerical Tools (2/4)

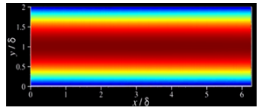


- Solves the neutron transport equation or the equivalent problem
- Two main methods are available for steady and transient calculations:
  - Deterministic approach using a SPN method
    - Two levels of discretization: SP_1 (≅ diffusion) and SP_3
    - Low computational cost but often fails to accurately predict the reactivity in small heterogeneous nuclear systems
    - Determination of the neutronics properties required by these models could be challenging in heterogeneous systems
  - Quasi-static Monte Carlo method
    - Monte Carlo method (first principles) provides high precision and flexibility for small and heterogeneous nuclear systems
    - Employs a quasi-static approach: flux is split as $\psi(\vec{r},\vec{\Omega},E,t) = n(t) \cdot \phi(\vec{r},\vec{\Omega},E,t)$ to decrease the computational resources needed during transient calculations
- Delayed neutron precursors concentrations (if liquid fuel) resolved by the thermal-hydraulics module
- As part of the design study, the module can be used to perform fuel burnup of shielding calculations

Numerical Tools (3/4)

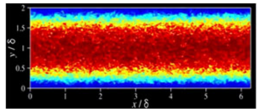


- Solves mass, momentum (Navier-Stokes equations) and energy balance equations in fluid and solid
- Both steady and transient calculations
- Uses existing Computational Fluid Dynamics (CFD) algorithms:
  - Navier-Stokes equations for laminar flow



Laminar
Re < ~2300

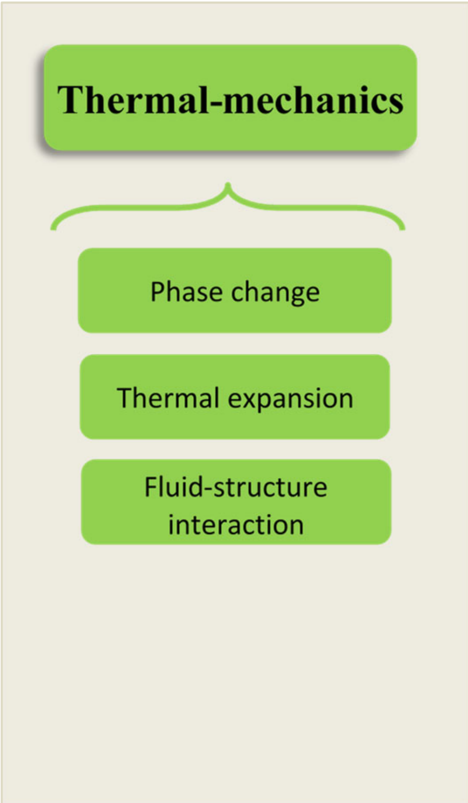
  - RANS (Reynolds average Navier-Stokes) approach for turbulent flow



Turbulent
Re > ~2300

  - More advanced turbulence models exist (LES, DNS)
  - Incompressible flow equations if low Mach number and small temperature gradients. Otherwise (e.g. pressure waves) compressible equations have to be used.
  - Two phase flow in some cases (e.g. MSFR draining)
- Energy conservation solved by considering:
  - Advection of flow internal energy
  - Internal power source from nuclear fissions and heat decay (liquid fuel)
  - Thermal radiation heat transfer in the fluid
  - Conjugated heat

Numerical Tools (4/4)



- Molten salt phase change phenomena:
  - **MASOFOAM** (MAcro-scale SOlification Foam): implements a solidification-convection coupled solver (mass, linear momentum and energy conservations) based on a mixture model (liquid phase, solid phase and the mushy zone)
  - **MUSOFOAM** (MUlti-scale SOlification Foam): improves the accuracy of the previous model by solving the species diffusion equation with a length adaptable phase field model. Provides MASOFOAM with properties averaged values (e.g. conductivity tensor for the solidified salt).
- Thermal expansion effects can be studied using a linear thermo-elasticity model for the solid regions:
  - Duhamel-Neumann relation
  - Momentum balance equation for the solid
  - Energy conservation (conduction + heat source)

Partners, Education & Training

- International collaborations and partners
  - SAMOFAR and SAMOSAFER Euratom H2020 projects: POLIMI and DELFT University
  - Institute Balseiro (Argentine): ARFITEC project
  - University of Texas (Texas A&M): NEST project
  - IAEA initiative: ONCORE (Open-source Nuclear Codes for Reactor Analysis)
- National collaborations
  - IRSN: criticality accidents (→2019)
  - EDF: corium-concrete interactions and uncertainties propagation (→ 2018)
  - CEA, ORANO and CNRS labs: ISAC (Innovative System for Actinides Conversion) Project (2022-2026)
- Education and Training
  - Training opportunities (since 2015): 17 internships, 7 PhDs and 3 Postdocs
  - New course: molten salts for energy applications (modeling + labs at FEST)

Activities and Funding

- Multiphysics numerical and experimental activities structured about four main topics:
    a) Molten Salt Fast Reactors
    b) Criticality and severe accidents
    c) Nuclear space propulsion
    d) Targets for neutron production

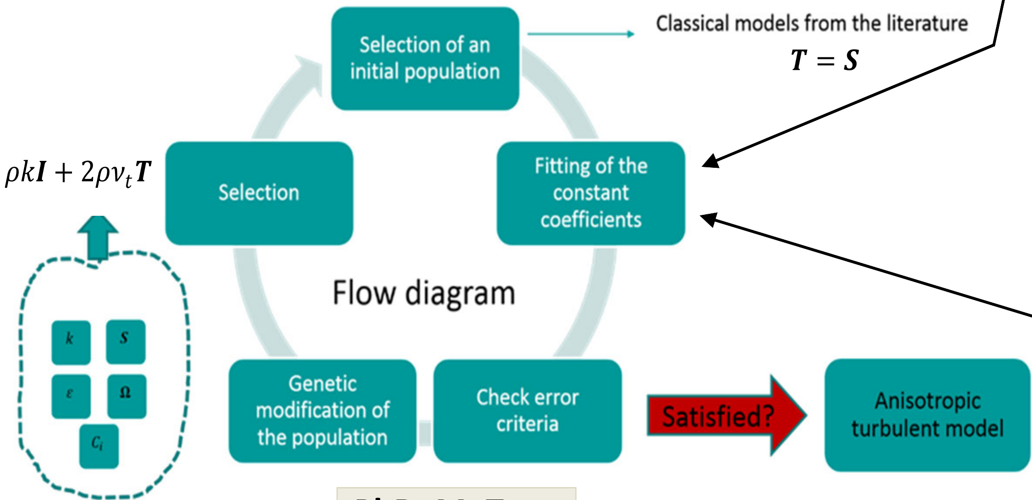
- Funding sources
    - H2020 Euratom projects SAMOFAR (2015-2019) and SAMOSAFER (2019-2023): are the principal funding source for the experiments
    - PhD and Postdoc positions funding:
        - ✓ Doctoral school, group internal funding and IN2P3
        - ✓ Collaboration with industry: IRSN and EDF

Numerical Activities

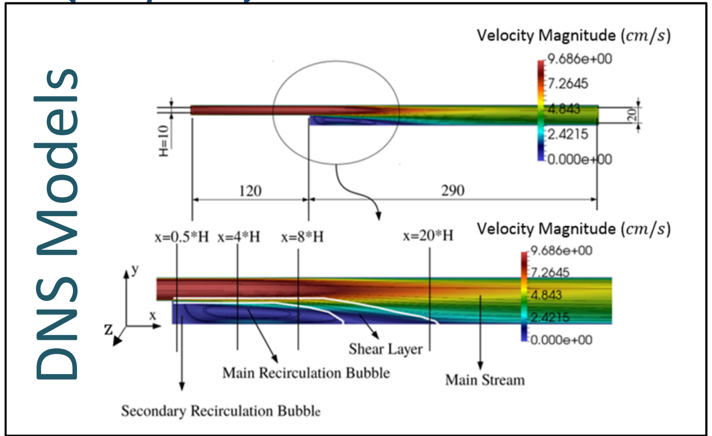
Molten Salt Fast Reactors (1/4)

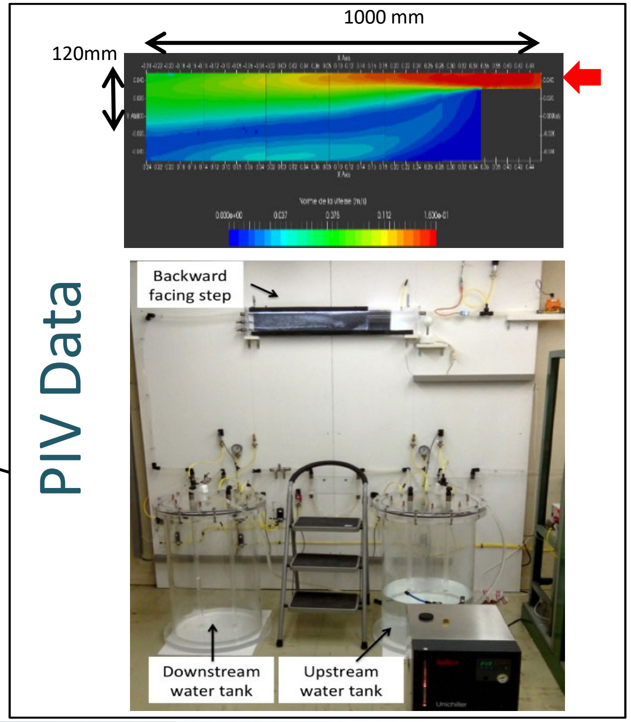
- Turbulence modeling for liquid fuel
  - Reynolds Average Navier Stokes (RANS) are well suited for multiphysics calculations but they can introduce significant errors (10–20%)
  - A tool based on a genetic algorithm was developed to construct a mathematical expression, using data from higher fidelity models (e.g. DNS) and experiments, to calculate the Reynolds Shear Stress (RSS) tensor
  - A RANS model was then developed from a BFS section

$$\boldsymbol{\tau}_{turb} = -\frac{2}{3}\rho k\boldsymbol{I} + 2\rho\nu_t\boldsymbol{T}$$



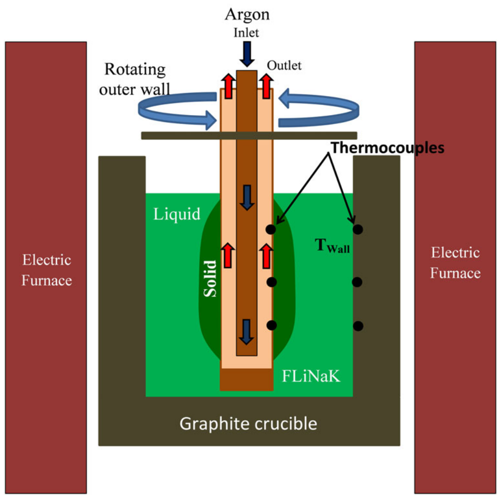
PhD. M. Tano (2015-2018)



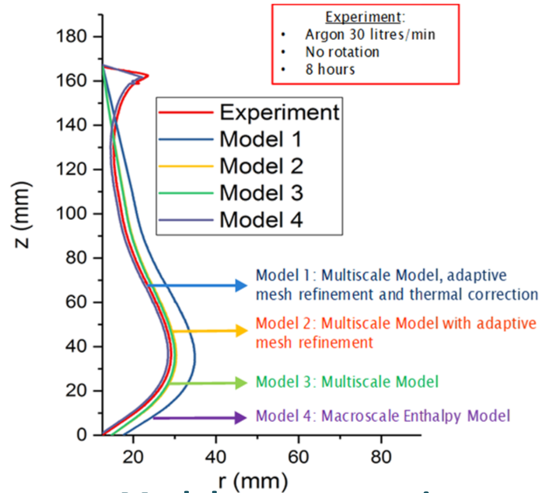


Molten Salt Fast Reactors (2/4)

- Salt phase change modeling
  - Possibility of undesirable fuel salt solidification in the fuel loop with complex solid phase morphology and properties
  - Solidification is a multiscale phenomenon. Two models were then developed:
    - **MASOFOAM** (MAcro-scale SOlification Foam)
    - **MUSOFOAM** (MUlti-scale SOlification Foam)
  - The accuracy of the solidification models developed for the ternary system Fli-KF-NaF was investigated in SWATH-S:
    - Rotating cooler tube inside an annular cavity filled with a molten salt
    - Good results only obtained when including convection and radiation effects



Experimental setup

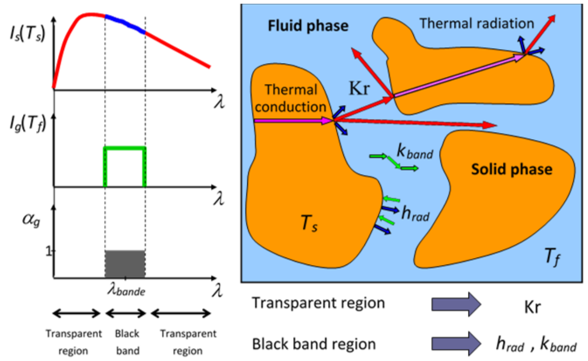


Model versus experiment

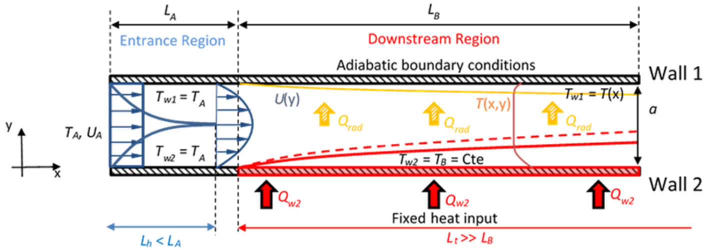
PhD. M. Tano (2015-2018)

Molten Salt Fast Reactors (3/4)

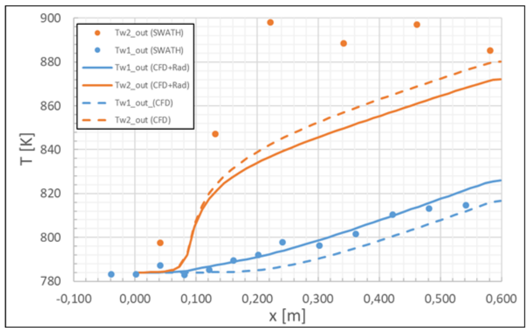
- Thermal radiation modeling
  - High temperature molten salts can be considered as a semi-transparent participative medium
  - A Black Band with a Surface to Surface (S2S) radiation model and the Rosseland approximation have been include in the energy balance equation
  - A flat Channel experiment has been developed to investigate thermal radiation heat transfer:
    - Based on the growth of the thermal Boundary Layer (BL) which depends on the optically thickness of the channel
    - Heat input to the flow is relative low
    - BL measured by thermocouples
  - The experimental results can be fitted by the simulation only if radiation heat transfer between the two walls is allowed



Thermal Radiation model for the salt



Flat Channel working principle

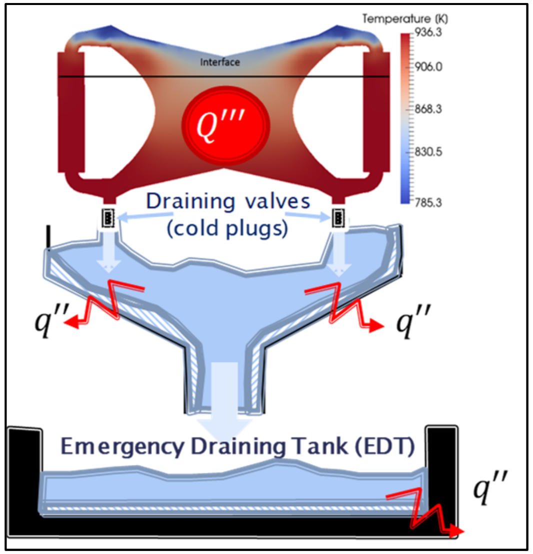


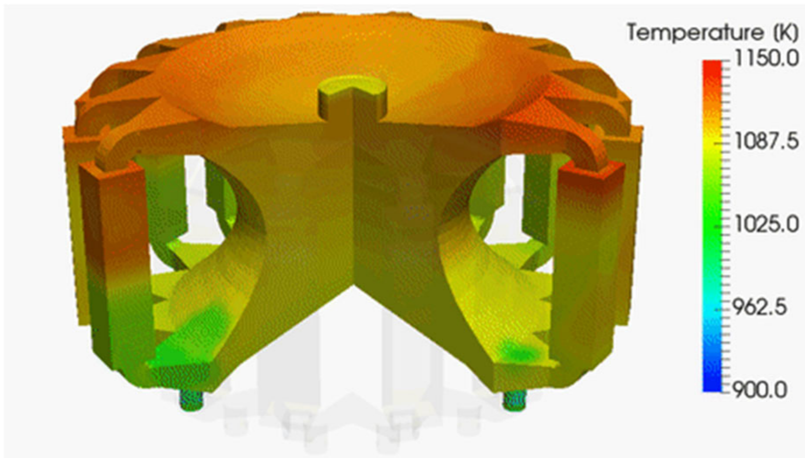
Model versus experiment results

Molten Salt Fast Reactors (4/4)

- MSFR draining model developed in the framework of the SAMOFAR project
- Initial event: Station blackout or total electric power failure (t = 0 sec)
- Draining of the fuel salt follows the opening of the draining valves (e.g. cold plugs melt)
- Numerical model:
  - ✓ Homogenized two phase model (mixture)
  - ✓ Fission power + residual heat
  - ✓ Incompressible flow
  - ✓ Boussinesq approximation
  - ✓ RSS RANS model
  - ✓ Salt solidification/melting (for the cold plug)
  - ✓ Radiative heat transfer
  - ✓ HXs modeled as porous medium
  - ✓ All fuel circuit walls are adiabatic (except HXs)

PhD. M. Tano (2015-2018)



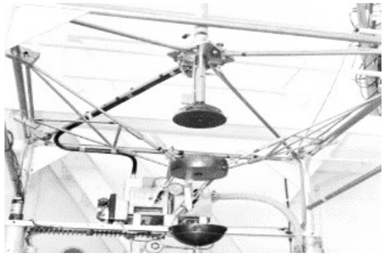


Criticality Accidents (1/2)

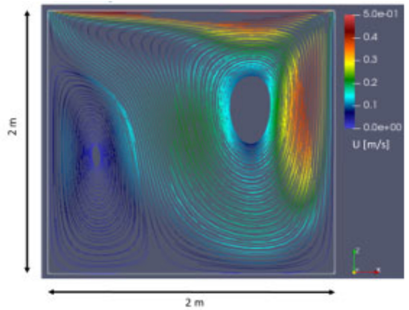
- Criticality accident: involuntary and uncontrolled fission chain reaction
- Collaboration with IRSN (PhD J. Blanco 2020)
- Goal: Development a general transient tool based on the multiphysics tool
  - Detailed phenomena modeling
  - Higher space/time scale flexibility
  - Best-Estimate (Not conservative)
- Cover a wide range of systems and phenomena:

Systems

Solid Media
- GODIVA
- Flattop

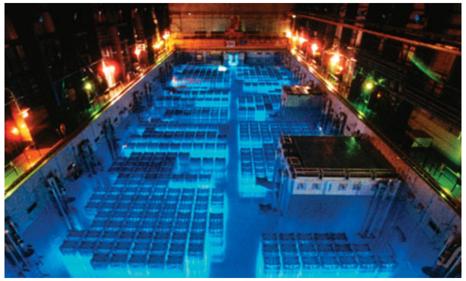


Liquid Media
- SILENE
- CNRS Cavity Benchmark



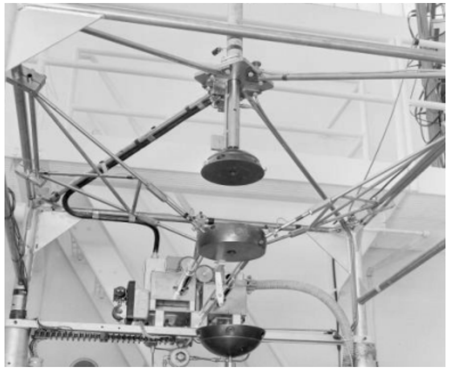
PhD. J. Blanco (2017-2020)

Heterogeneous Media (Solid-Liquid)
- Spent Fuels Pools
- Research reactors

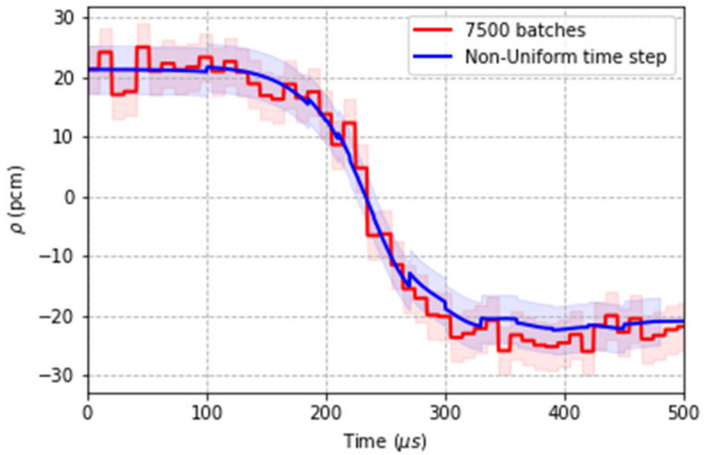


Criticality Accidents (2/2)

- Two transient neutronics models were developed: SPN and Quasi-Static Monte Carlo (QS-MC)
- Godiva reactor experiments were used to evaluated these neutronics methods
  - High enriched Uranium (95%) sphere (~8.85 cm radius)
  - The prompt-burst was initiated by a quick reactivity insertion
  - Thermal expansion increase neutron leakage thus decreasing reactivity
  - Very good results obtained with the Monte Carlo Quasi-static using a non-uniform time step for the flux shape calculation

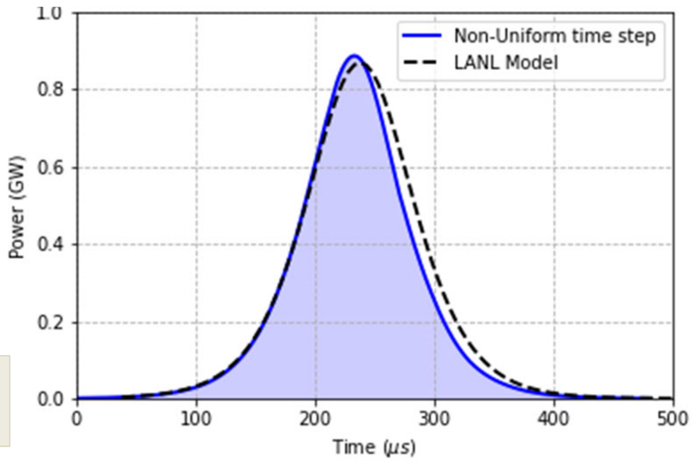


Godiva Reactor



QS-MC Uniform versus Non-uniform time steps

PhD. J. Blanco (2017-2020)



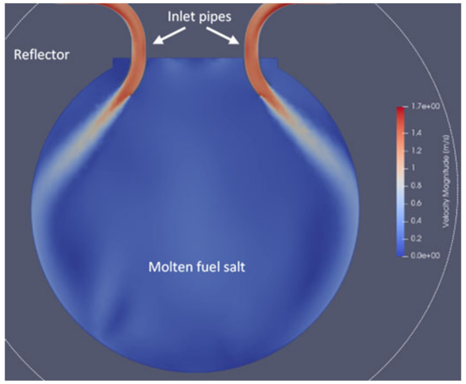
Prompt neutrons power peak during the transient

Nuclear Space Propulsion (1/2)

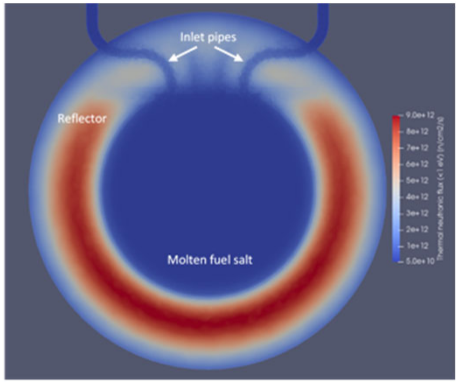
- Nuclear fission power is expected to play a key role in space exploration in the coming years
- Molten Salt Reactors (MSRs) offer some intrinsic advantages for Nuclear Electric Propulsion (NEP)
  - High power densities and temperatures
  - Lower fuel pressure and temperature gradients
  - Potentially simple reactivity control systems
- Design work of a space MSR poses technical challenges
  - Issues related to materials damage by neutrons and salt corrosion
  - Power conversion system and radiator designs
  - Nuclear tests and system integration
  - Small reactor system with very high coupled phenomena
- NEP reactors are also suitable systems for multiphysics models

Nuclear Space Propulsion (2/2)

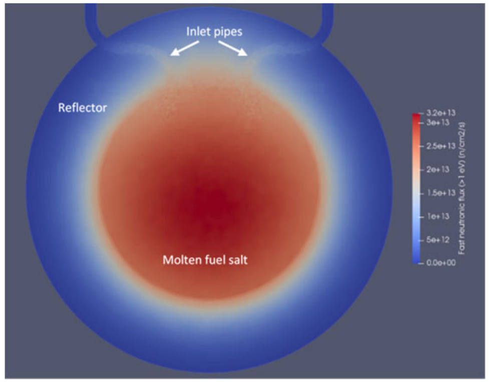
- Preliminary results:
  - Fast MSR using LEU LiF-UF_4 and Beryllium reflector



Molten fuel salt velocity



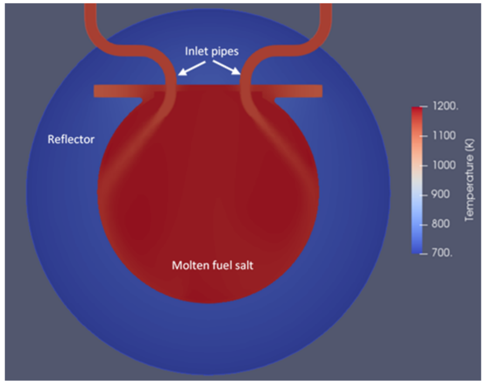
Thermal neutron flux (< 1eV)



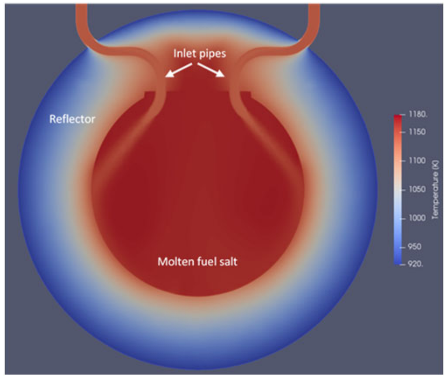
Fast neutron flux (>1 eV)

- Design evaluation: thermal control of the reflector

PhD. F. Quinteros (2020-2023)



Temperature field (with insulation)



Temperature field (no insulation)

Conclusions

- Use of multi-physics approaches in the nuclear industry and academia will continue to increase in the coming years
  - Novel applications are currently being investigated
  - These approaches will be key to improve the design of current NPPs, advanced reactors designs (MMR, SMR, etc.) and novel nuclear fuels
  - Nevertheless a multi-physics tool is not always the more efficient approach !
- More international collaborative frameworks are needed to continue developing and sharing these new tools and methods
  - Example: Open-Source Nuclear Codes for Reactor Analysis (ONCORE)

Perspectives (5 years)

- MSR modeling:
  - SAMOSAFER (2019-2023): Completing tasks (open channel and natural convection)
  - ISAC (2022-2026): Develop an experimental and numerical study of the production, transport and separation of fission products in the molten fuel salt circuit

- Space propulsion:
  - Complete MSR fast and thermal concepts conceptual designs (2020-2025)
  - Enhance the exiting tool to include other reactors such as Heat Pipe Reactors (HPRs)
  - Pursue collaborations with international and national partners

- Criticality accidents
  - Use the multiphysics tool to study criticality accidents in other systems
  - Continue the collaboration with the IRSN

Thank you !