Deterministic modelling of nuclear systems

Spring School on Sodium Cooled Fast Reactors

University of Cambridge, March 29th-31st, 2021 – online

Prof. Christophe Demazière
demaz@chalmers.se

@ChrisDemaz

DREAM

TASK FORCE ON
DETERMINISTIC REACTOR MODELLING

Structure of the presentation

- Introduction
- Reminder about the local balance equations in neutronics and thermal-hydraulics
- Derivation of the coarse mesh balance equations
- Closing the system of equations
- Solving the system of equations

Introduction

Introduction

- Nuclear reactor systems = **large** and **complex** systems
- Strongly **heterogeneous** systems, especially for the core, with **different scales**, by **design** and due to the **physical phenomena** involved, such as:
  - **Neutron interactions** at the **atomic** scale
  - **Turbulence** and **boiling** at the **millimeter** scale
  - **Pins** at the **centimeter** scale
  - **Assembly** at the **decimeter** scale
  - **Core** at the **meter** scale

➢ **Multi-scale** and **multi-physics** systems

➢ Strangely enough for the neutronics, the **deterministic** modelling of such systems relies on the principles of **continuum physics**

Introduction

- How to model such systems?

… the large size requires a **coarse mesh** modelling

… phenomena at the **local scales** influence the **global scales**

➢Need to construct a modelling framework **preserving the multi-scale phenomena** while **only resolving the global <u>multi-physics</u> problem**

➢Lecture focusing on **neutronics** and **thermal-hydraulics**

- **Disclaimer**: lecture focusing on the rational behind the modelling approach rather than on how the modelling is done

Reminder about the local balance equations

Reminder about the local balance equations in neutronics

- Local balance equations in **neutronics** given by the **neutron transport equation** or **Boltzmann equation**:

$$\frac{1}{v(E)}\frac{\partial}{\partial t}\psi(\mathbf{r},\mathbf{\Omega},E,t)+\mathbf{\Omega}\cdot\nabla\psi(\mathbf{r},\mathbf{\Omega},E,t)+\Sigma_t(\mathbf{r},E,t)\psi(\mathbf{r},\mathbf{\Omega},E,t)$$
$$=\int_{(4\pi)}\int_0^\infty \Sigma_s(\mathbf{r},\mathbf{\Omega}'\to\mathbf{\Omega},E'\to E,t)\psi(\mathbf{r},\mathbf{\Omega}',E',t)d^2\mathbf{\Omega}'dE'$$
$$+\frac{\chi^p(\mathbf{r},E)}{4\pi}\left[1-\tilde{\beta}(\mathbf{r})\right]\int_0^\infty \nu(\mathbf{r},E')\Sigma_f(\mathbf{r},E',t)\phi(\mathbf{r},E',t)dE'+\frac{1}{4\pi}\sum_{i=1}^{N_d}\chi_i^d(\mathbf{r},E)\lambda_i(\mathbf{r})C_i(\mathbf{r},t)$$

with

$$\frac{\partial C_i}{\partial t}(\mathbf{r},t)dt=\tilde{\beta}_i(\mathbf{r})\int_0^\infty \nu(\mathbf{r},E)\Sigma_f(\mathbf{r},E,t)\phi(\mathbf{r},E,t)dE-\lambda_i(\mathbf{r})C_i(\mathbf{r},t),i=1,\ldots,N_d$$

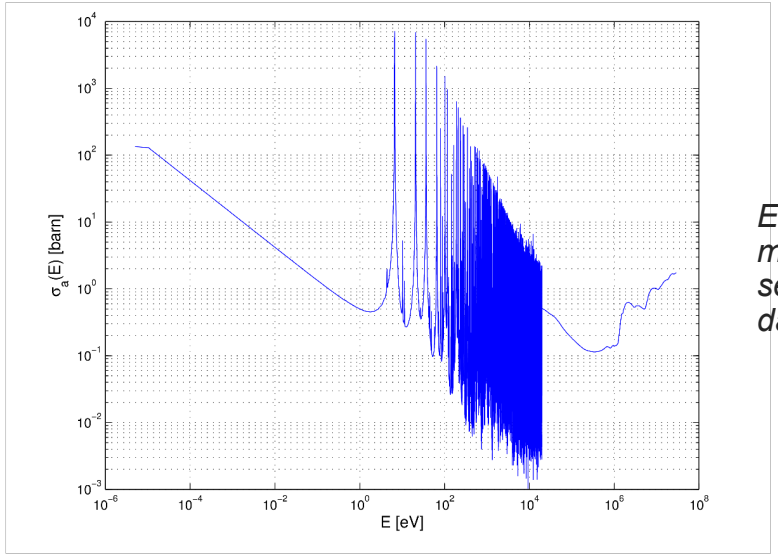
Reminder about the local balance equations in neutronics

- **Complex** equations:
  - **Integro-differential** equations
  - **Multi-dimensional phase space** for the variable, i.e. $\left(\mathbf{r}, \mathbf{\Omega}, E, t\right)$
  - The **macroscopic cross-section data**, defined as:

$$\Sigma_{\alpha}\left(\mathbf{r}, E, t\right) = \sum_{X} N_{X}\left(\mathbf{r}, t\right) \sigma_{\alpha X}\left(E\right)$$

  have a **complex dependence on energy**

Reminder about the local balance equations in neutronics



Energy-dependence of the microscopic absorption cross-section for ^{238}U (JEFF 3.1 neutron data library)

$1/v$ -behaviour region

resonance region

continuum region

resolved resonances

unresolved resonances

Reminder about the local balance equations in thermal-hydraulics

- Local balance equations in **thermal-hydraulics** given:
  - In the **fluid**, by the **Navier-Stokes equations** complemented by an "**energy**" **conservation equation**:

$$\frac{\partial \rho}{\partial t}(\mathbf{r},t) + \boldsymbol{\nabla} \cdot (\rho \mathbf{v})(\mathbf{r},t) = 0$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t}(\mathbf{r},t) + \boldsymbol{\nabla} \cdot (\rho \mathbf{v} \otimes \mathbf{v})(\mathbf{r},t) = \boldsymbol{\nabla} \cdot \boldsymbol{\tau}(\mathbf{r},t) - \boldsymbol{\nabla} P(\mathbf{r},t) + \rho(\mathbf{r},t)\mathbf{g}$$

$$\rho(\mathbf{r},t)\frac{\partial h}{\partial t}(\mathbf{r},t) + (\rho \mathbf{v})(\mathbf{r},t) \cdot \boldsymbol{\nabla} h(\mathbf{r},t) = -\boldsymbol{\nabla} \cdot \mathbf{q}''(\mathbf{r},t) + q'''(\mathbf{r},t) + \boldsymbol{\tau}(\mathbf{r},t) : \left[\boldsymbol{\nabla} \otimes \mathbf{v}(\mathbf{r},t)\right] + \frac{\partial P}{\partial t}(\mathbf{r},t) + \mathbf{v}(\mathbf{r},t) \cdot \boldsymbol{\nabla} P(\mathbf{r},t)$$

  - In the **solids**, by the **heat conduction equation**:

$$c_P(\mathbf{r},t)\rho(\mathbf{r},t)\frac{\partial T}{\partial t}(\mathbf{r},t) = q'''(\mathbf{r},t) + \boldsymbol{\nabla} \cdot \left[k(\mathbf{r},t)\boldsymbol{\nabla} T(\mathbf{r},t)\right]$$

Reminder about the local balance equations in thermal-hydraulics

- Local balance equations in **thermal-hydraulics** complemented by:
  - **Equation of state** for the **fluid**, such as:

$$\rho\left(\mathbf{r},t\right) \equiv \rho\left[P\left(\mathbf{r},t\right),h\left(\mathbf{r},t\right)\right]$$

  - **Constitutive equations** for the **fluid**, such as:

$$\boldsymbol{\tau}\left(\mathbf{r},t\right) \equiv \boldsymbol{\tau}\left[P\left(\mathbf{r},t\right),h\left(\mathbf{r},t\right),\mathbf{v}\left(\mathbf{r},t\right)\right]$$

$$\mathbf{q}''\left(\mathbf{r},t\right) \equiv \mathbf{q}''\left[P\left(\mathbf{r},t\right),h\left(\mathbf{r},t\right),T\left(\mathbf{r},t\right)\right]$$

  - **Constitutive equations** for the **solids**, such as:

$$c_P\left(\mathbf{r},t\right) \equiv c_P\left[T\left(\mathbf{r},t\right)\right]$$

$$\rho\left(\mathbf{r},t\right) \equiv \rho\left[T\left(\mathbf{r},t\right)\right]$$

$$k\left(\mathbf{r},t\right) \equiv k\left[T\left(\mathbf{r},t\right)\right]$$

Reminder about the local balance equations in thermal-hydraulics

- Note about the **constitutive** equations:
  - The **constitutive** equations are based either on **first principles** or **phenomenological principles**
  - Obtaining such equations often relies on **experiments**
  - ➢Such constitutive equations thus often depend on the **specific conditions on the experiments**

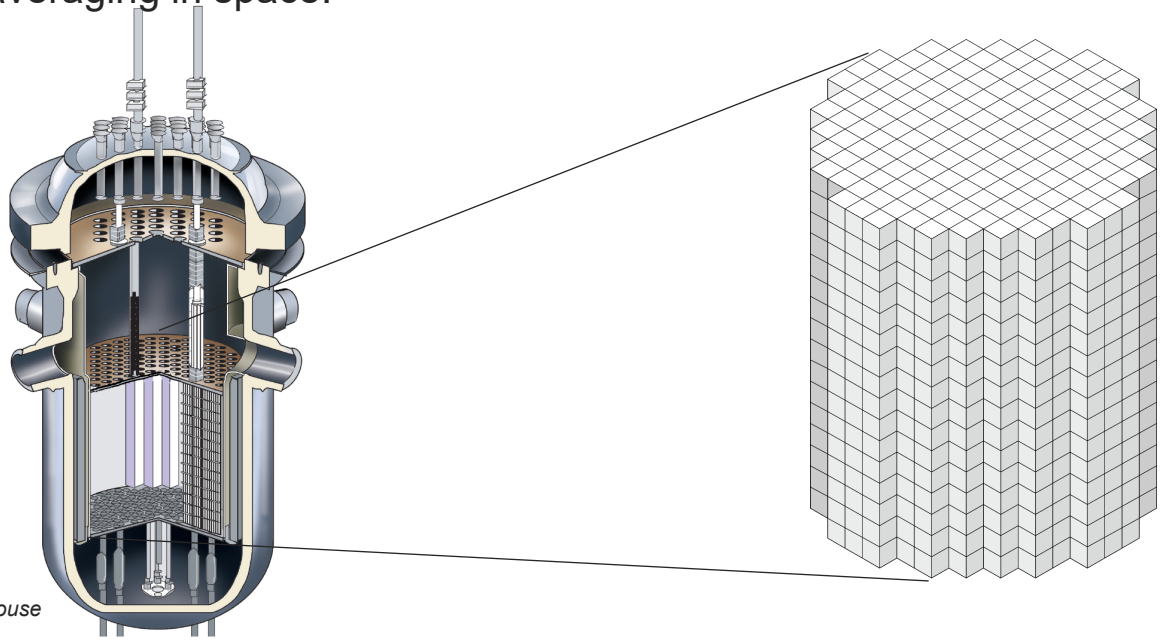
Coarse mesh balance equations

Coarse mesh balance equations

- Due to the **complexity** of the systems and their **size**, need to **average** the local balance equations on a proper **multi-dimensional grid**:
  - For the **neutronics**:
    - Average in **space** (homogenization)
    - Average in **angle**
    - Average in **energy** (condensation)
  - For the **thermal-hydraulics**:
    - Average in **space**
    - Average in **time**

Coarse mesh balance equations

- Example of the averaging in space:



Picture courtesy of Westinghouse Electric Sweden AB

Coarse mesh balance equations

- The averaging of the equations need to **preserve "meaningful" quantities**, so that solving the averaged equations lead to the true averages of the quantities of interest

➢ **Far from trivial task**, especially for the neutronics

Coarse mesh balance equations in neutronics

- Average in **angle**: in essence, procedure equivalent to:
  - **Integrating** the transport equation on **all solid angles**
  - Replacing the **isotropic scattering cross-section** by its **transport corrected value**:

$$\Sigma_{s0}\left(\mathbf{r}, E' \to E\right) - \delta\left(E' - E\right)\int_0^\infty \Sigma_{s1}\left(\mathbf{r}, E' \to E\right) dE$$

  - Solving for the **scalar neutron flux**:

$$\phi\left(\mathbf{r}, E, t\right) = \int_{(4\pi)} \psi\left(\mathbf{r}, \mathbf{\Omega}, E, t\right) d^2\mathbf{\Omega}$$

    and for the **neutron current density vector**:

$$\mathbf{J}\left(\mathbf{r}, E, t\right) = \int_{(4\pi)} \mathbf{\Omega}\psi\left(\mathbf{r}, \mathbf{\Omega}, E, t\right) d^2\mathbf{\Omega}$$

  - Assume **proportionality** between the **neutron current density vector** and the **gradient of the scalar neutron flux** (Fick's law):

$$\mathbf{J}\left(\mathbf{r}, E, t\right) = -D\left(\mathbf{r}, E, t\right)\mathbf{\nabla}\phi\left(\mathbf{r}, E, t\right)$$

Coarse mesh balance equations in neutronics

- Average in **angle**: in essence, procedure equivalent to:
  - Note: A **more rigorous approach** is to first derive the so-called P_1 approximation of the transport equation and to assume equal anisotropic in-scatter and out-scatter at every energy

➢Obtained balance equations:

$$\frac{1}{v(E)}\frac{\partial\phi}{\partial t}(\mathbf{r},E,t)=\nabla\cdot\left[D(\mathbf{r},E,t)\nabla\phi(\mathbf{r},E,t)\right]+\int_0^\infty\Sigma_{s0}(\mathbf{r},E'\to E,t)\phi(\mathbf{r},E',t)dE'$$
$$+\frac{\left[1-\tilde{\beta}(\mathbf{r})\right]\chi(\mathbf{r},E)}{k}\int_0^\infty\nu(\mathbf{r},E')\Sigma_f(\mathbf{r},E',t)\phi(\mathbf{r},E',t)dE'+\sum_{i=1}^{N_g}\lambda_i(\mathbf{r})\chi_{i,g}^d(\mathbf{r})C_i(\mathbf{r},t)-\Sigma_t(\mathbf{r},E)\phi(\mathbf{r},E)$$

and

$$\frac{\partial C_i}{\partial t}(\mathbf{r},t)dt=\tilde{\beta}_i(\mathbf{r})\int_0^\infty\nu(\mathbf{r},E)\Sigma_f(\mathbf{r},E,t)\phi(\mathbf{r},E,t)dE-\lambda_i(\mathbf{r})C_i(\mathbf{r},t),i=1,\ldots,N_d$$

Coarse mesh balance equations in neutronics

- Average in **energy**:
  - The neutron energy range of interest $\left[E_{min};E_{max}\right]$ is divided into G adjacent **energy groups**:

$$\left[E_{min};E_{max}\right]=\bigcup_{g=G}^{1}\left[E_g;E_{g-1}\right]$$

  - All energy-dependent quantities are **integrated with respect to energy** on such energy groups using proper **weighting functions**

- Obtained balance equations:

$$\frac{1}{v_g}\frac{\partial\phi_g}{\partial t}\left(\mathbf{r},t\right)=\nabla\cdot\left[D_g\left(\mathbf{r},t\right)\nabla\phi_g\left(\mathbf{r},t\right)\right]+\sum_{g'=1}^{G}\Sigma_{s0,g'\to g}\left(\mathbf{r},t\right)\phi_{g'}\left(\mathbf{r},t\right)$$

$$+\left[1-\tilde{\beta}\left(\mathbf{r}\right)\right]\chi_g^p\left(\mathbf{r}\right)\sum_{g'=1}^{G}\nu_{g'}\left(\mathbf{r}\right)\Sigma_{f,g'}\left(\mathbf{r},t\right)\phi_{g'}\left(\mathbf{r},t\right)+\sum_{i=1}^{N_g}\lambda_i\left(\mathbf{r}\right)\chi_{i,g}^d\left(\mathbf{r}\right)C_i\left(\mathbf{r},t\right)-\Sigma_{t,g}\left(\mathbf{r},t\right)\phi_g\left(\mathbf{r},t\right)$$

and

$$\frac{\partial C_i}{\partial t}\left(\mathbf{r},t\right)=\tilde{\beta}_i\left(\mathbf{r}\right)\sum_{g'=1}^{G}\nu_{g'}\left(\mathbf{r}\right)\Sigma_{f,g'}\left(\mathbf{r},t\right)\phi_{g'}\left(\mathbf{r},t\right)-\lambda_i\left(\mathbf{r}\right)C_i\left(\mathbf{r},t\right),i=1,\ldots,N_d$$

Coarse mesh balance equations in neutronics

- Average in **space**:
  - Quantities to be solved for:
    - **Volume-averaged scalar neutron flux**: $\phi_{g,n}(t) = \frac{1}{V_n}\int_{V_n} \phi_g(\mathbf{r},t) d^3\mathbf{r}$
    - **Surface-averaged net neutron current** along the direction $\aleph$: $J^{\aleph}_{g,n}(t) = \frac{1}{S^{\aleph}_n}\int_{S^{\aleph}_n} \mathbf{J}_g(\mathbf{r},t).\mathbf{N}_{\aleph} d^2\mathbf{r}$

➢Obtained balance equations (in cartesian coordinate system):

$$\frac{1}{v_g}\frac{\partial \phi_{g,n}}{\partial t}(t) = -\sum_{\aleph=x,y,z} \frac{J^{\aleph}_{g,n}(t) - J^{\aleph}_{g,n-1}(t)}{\Delta\aleph} - \Sigma_{t,g,n}(t)\phi_{g,n}(t) + \sum_{g'=1}^{G} \Sigma_{s0,g'\to g,n}(t)\phi_{g',n}(t)$$

$$+\chi^{p}_{g,n}\left(1-\tilde{\beta}_n\right)\sum_{g'=1}^{G}\nu_{g',n}\Sigma_{f,g',n}(t)\phi_{g',n}(t) + \sum_{i=1}^{N_d}\chi^{d}_{i,g,n}\lambda_{i,n}C_{i,n}(t)$$

and

$$\frac{\partial C_{i,n}}{\partial t}(t) = \tilde{\beta}_{i,n}\sum_{g'=1}^{G}\nu_{g',n}\Sigma_{f,g',n}(t)\phi_{g',n}(t) - \lambda_{i,n}C_{i,n}(t), i = 1,\ldots,N_d$$

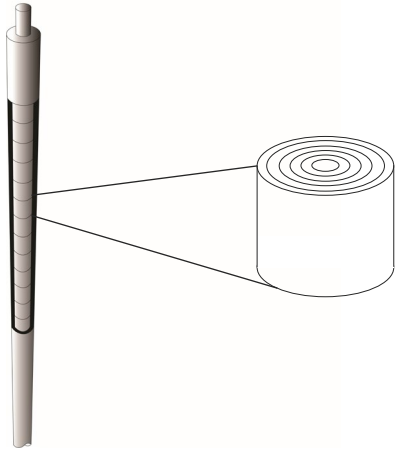
Coarse mesh balance equations in thermal-hydraulics

- Average in **space**:
  - For the **heat conduction equations** in **solids**:

    Partitioning of the fuel pins in **axial** and **radial** layers:

    Volume integration of the heat conduction equation:

$$\frac{1}{V_i}\int_V \rho(\mathbf{r},t)c_p(\mathbf{r},t)\frac{\partial T}{\partial t}(\mathbf{r},t)d^3\mathbf{r} = \frac{1}{V_i}\int_{S_i} k(\mathbf{r},t)\nabla T(\mathbf{r},t)\cdot\mathbf{N}d^2\mathbf{r} + \frac{1}{V_i}\int_{V_i} q'''(\mathbf{r},t)d^3\mathbf{r}$$



Picture courtesy of the Swedish Academic Initiative for Radiation Sciences and Nuclear Technology

Coarse mesh balance equations in thermal-hydraulics

- Average in **space**:
  - For the **fluid**:

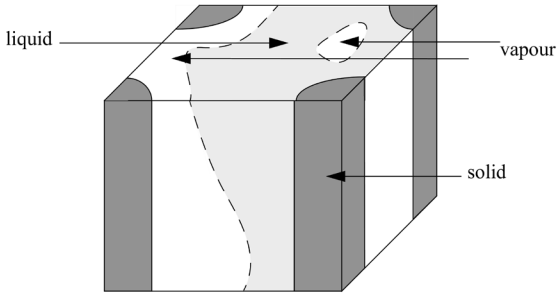
    Use of the **phase density function**:

$$\text{At time } t,\ \alpha_k\left(\mathbf{r},t\right)=\begin{cases}1 \text{ if } \mathbf{r}\in \text{phase } k\\ 0 \text{ if } \mathbf{r}\notin \text{phase } k\end{cases}$$

    Volume integration on the **sub-volumes** occupied by either the **liquid phase** ($k\equiv l$) or the **vapour phase** ($k\equiv v$)

➢ Two types of averages introduced:

- One-phase average: $\left\langle c_k\right\rangle_k=\dfrac{1}{D_k}\displaystyle\int_{D_k} c_k\left(\mathbf{r},t\right)d^n\mathbf{r}$
- Two-phase average: $\left\langle c\right\rangle=\dfrac{1}{D}\displaystyle\int_{D} c\left(\mathbf{r},t\right)d^n\mathbf{r}$



Coarse mesh balance equations in thermal-hydraulics

- Average in **space**:
  - For the **fluid**:

    Obtained balance equations written in a generic sense and for scalar quantities f:

$$\frac{\partial}{\partial t}\left[\beta\left\langle\alpha_k\right\rangle\left\langle\rho_k f_k\right\rangle_k\right]+\nabla\cdot\left[\beta\left\langle\alpha_k\right\rangle\left\langle\rho_k f_k \mathbf{v}_k\right\rangle_k\right]=\beta\left\langle\alpha_k\right\rangle\left\langle\rho_k \theta_k\right\rangle_k-\nabla\cdot\left[\beta\left\langle\alpha_k\right\rangle\left\langle\mathbf{\Phi}_k\right\rangle_k\right]-\frac{1}{V}\int_{S_{ki}}\left[\rho_k f_k\left(\mathbf{v}_k-\mathbf{v}_S\right)+\mathbf{\Phi}_k\right]\cdot\mathbf{N}d^2\mathbf{r}-\frac{1}{V}\int_{S_{kw}}\mathbf{\Phi}_k\cdot\mathbf{N}d^2\mathbf{r}$$

	Conservation of mass	Conservation of momentum	Conservation of energy
f or $\mathbf{f}$	1	$\mathbf{v}$	e
$\mathbf{\Phi}$	$\mathbf{0}$	$-\left(\boldsymbol{\tau}-P\mathbf{I}\right)$	$\mathbf{q}''-\left(\boldsymbol{\tau}-P\mathbf{I}\right)\cdot\mathbf{v}$
θ or $\boldsymbol{\theta}$	0	$\mathbf{g}$	$\frac{q'''}{\rho}+\mathbf{g}.\mathbf{v}$

➢ **Spatial averaging** equivalent to a **filtering** of the **small-scale** phenomena

Coarse mesh balance equations in thermal-hydraulics

- Average in **time** (only for the **fluid**):
  - Two type of averages introduced:
    - Time-average on Δt: $\underline{c} = \frac{1}{\Delta t}\int_{t-\frac{\Delta t}{2}}^{t+\frac{\Delta t}{2}} c\left(\mathbf{r},t\right)dt$
    - Time-average on Δt_k: $\underline{\underline{c}} = \frac{1}{\Delta t_k}\int_{t-\frac{\Delta t_k}{2}}^{t+\frac{\Delta t_k}{2}} c\left(\mathbf{r},t\right)dt$
  - Obtained balance equations written in a generic sense and for scalar quantities f:

$$\frac{\partial}{\partial t}\left[\beta\left\langle\underline{\alpha_k}\left(\underline{\underline{\rho_k f_k}}\right)\right\rangle\right] + \boldsymbol{\nabla}\cdot\left[\beta\left\langle\underline{\alpha_k}\left(\underline{\underline{\rho_k f_k \mathbf{v}_k}}\right)\right\rangle\right] = \beta\left\langle\underline{\alpha_k}\left(\underline{\underline{\rho_k \theta_k}}\right)\right\rangle - \boldsymbol{\nabla}\cdot\left[\beta\left\langle\underline{\alpha_k}\,\underline{\underline{\boldsymbol{\Phi}_k}}\right\rangle\right] - \underline{\frac{1}{V}\int_{S_{ki}}\left[\rho_k f_k\left(\mathbf{v}_k - \mathbf{v}_S\right) + \boldsymbol{\Phi}_k\right]\cdot\mathbf{N}\,d^2\mathbf{r}} - \underline{\frac{1}{V}\int_{S_{kw}}\boldsymbol{\Phi}_k\cdot\mathbf{N}\,d^2\mathbf{r}}$$

➢ **Time averaging** equivalent to a **filtering** of the **high-frequency** phenomena

Coarse mesh balance equations

- For the **neutronics**:
  - Need to chose a proper **spatial discretization scheme**
  - If **steady-state conditions** assumed: **eigenvalue problem** by renormalizing the fission source term by k_{eff}

    If **time-dependence**: need to chose a proper **time discretization scheme**
- For the **thermal-hydraulics**:
  - Need to simultaneously chose a proper **spatial discretization scheme** and **time discretization scheme**

“Closing” the coarse mesh equations

Macroscopic cross-section generation in neutronics

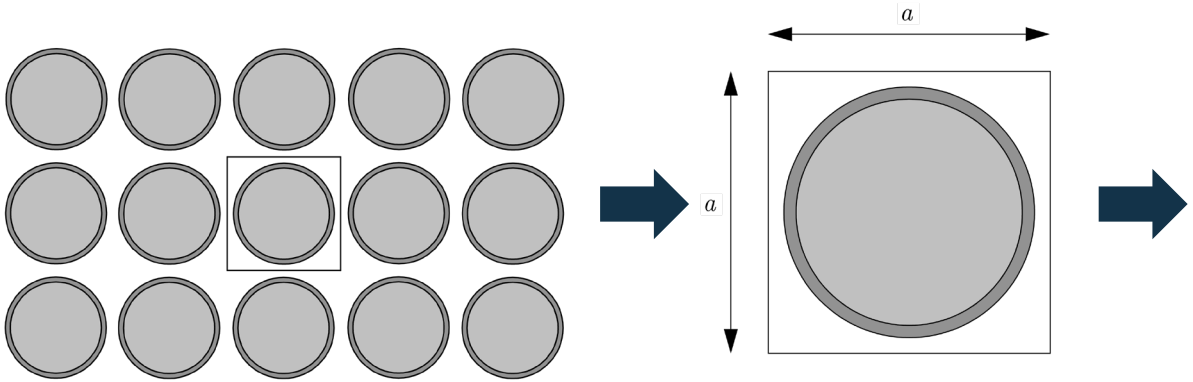
- "**Multi-scale**" approach followed:
  1. Choice of a **typical neutron spectrum** $\phi_w(E)$
  2. **Condensation** of the microscopic cross-sections on a **micro-energy group** structure:

$$\sigma_{\alpha X,g} = \frac{\int_{E_g}^{E_{g-1}} \sigma_{\alpha X}(E)\phi_w(E)dE}{\int_{E_g}^{E_{g-1}} \phi_w(E)dE}$$

Note: A **special treatment** is required for **resonant species** (not detailed here)

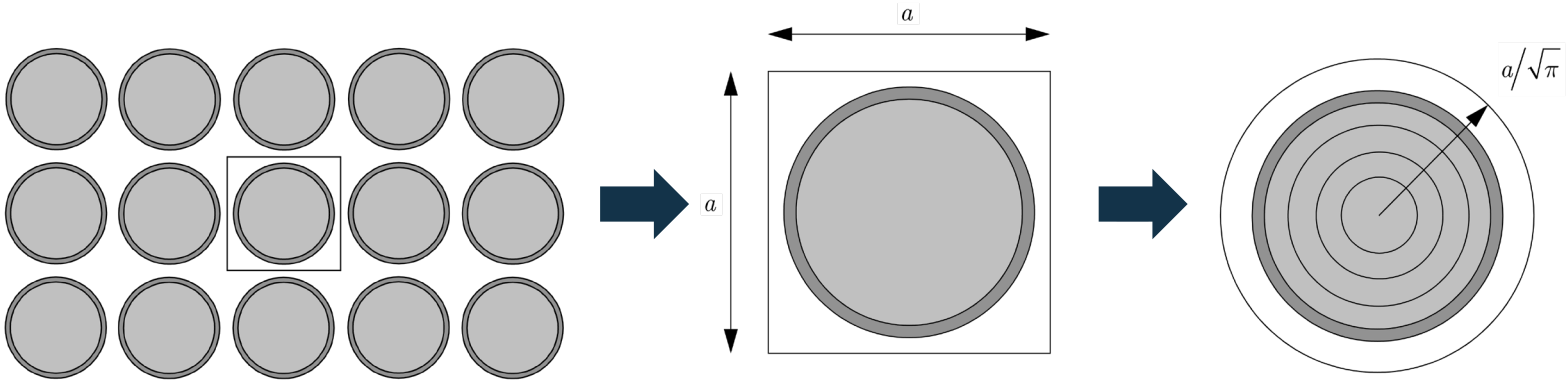
Macroscopic cross-section generation in neutronics

- "**Multi-scale**" approach followed:
  3. **Small subsystem** considered, with **micro-regions** used for the **spatial discretization**



Macroscopic cross-section generation in neutronics

- "**Multi-scale**" approach followed:
  3. **Small subsystem** considered, with **micro-regions** used for the **spatial discretization**



Resulting in: $\Sigma_{\alpha,i,g} = \sum_{X} N_{X,i} \sigma_{\alpha X,g}$

Macroscopic cross-section generation in neutronics

- "**Multi-scale**" approach followed:
  4. **Neutron transport** equation solved on the **micro-energy groups** g and **micro-regions** i for the **subsystem** with **proper boundary conditions**

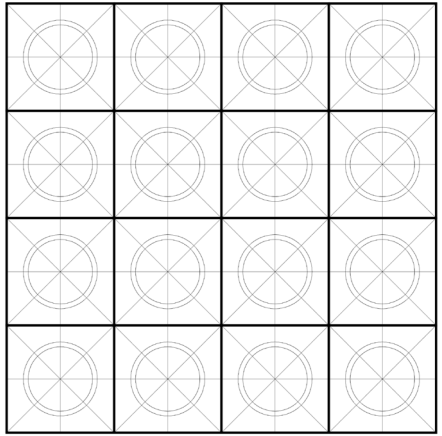
     resulting in $\phi_{i,g}$
  5. **Bigger subsystem** considered, with **macro-regions** used for the **spatial discretization** and **macro-groups** used for the **energy discretization**

     ➢**Condensation** of the macroscopic cross-sections:

$$\Sigma_{\alpha,i,G} = \frac{\sum_{g \in G} \Sigma_{\alpha,i,g} \phi_{i,g}}{\sum_{g \in G} \phi_{i,g}}$$

     ➢**Homogenization** of the macroscopic cross-sections:

$$\Sigma_{\alpha,I,G} = \frac{\sum_{i \in I} \Sigma_{\alpha,i,G} V_i \phi_{i,G}}{\sum_{i \in I} V_i \phi_{i,G}}$$



Macroscopic cross-section generation in neutronics

- "**Multi-scale**" approach followed:
  6. **Neutron transport** equation solved on the **macro-energy groups** G and **macro-regions** I for the **subsystem** with **proper boundary conditions**

     resulting in $\phi_{I,G}$
  7. **Condensation** and **homogenization** of the macroscopic cross-sections using the **macro-flux** $\phi_{I,G}$ on a multi-dimensional **mesh compatible** with the one of the **core simulator**
  8. Estimation of the **critical spectrum** ϕ_{G_B} in the subsystem
  9. **Re-balancing** of the **macro-flux** $\phi_{I,G}$ on the **critical spectrum** ϕ_{G_B} :

$$\phi_{I,G}^{L} = \frac{\sum_{G_B \in G} \phi_{G_B}}{\phi_G} \phi_{I,G} \qquad \text{with} \qquad \phi_G = \frac{\sum_I \phi_{I,G} V_I}{\sum_I V_I}$$

Macroscopic cross-section generation in neutronics

- "**Multi-scale**" approach followed:
  10. **Superimposition** of the **re-balanced macro-flux** $\phi^L_{I,G}$ on the **micro-flux** $\phi_{i,g}$:

$$\phi^L_{i,g} = \frac{V_I \phi^L_{I,G}}{\sum_{i' \in I} V_{i'} \sum_{g' \in G} \phi_{i',g'}} \phi_{i,g}$$

  11. **Rescaling** to the actual **power level** P of the system:

$$\phi^{L,P}_{i,g} = \frac{P}{\sum_{i'} V_{i'} \sum_{g'} \phi^L_{i',g'} \sum_X \kappa_X N_{X,i'} \sigma_{fX,i',g'}} \phi^L_{i,g}$$

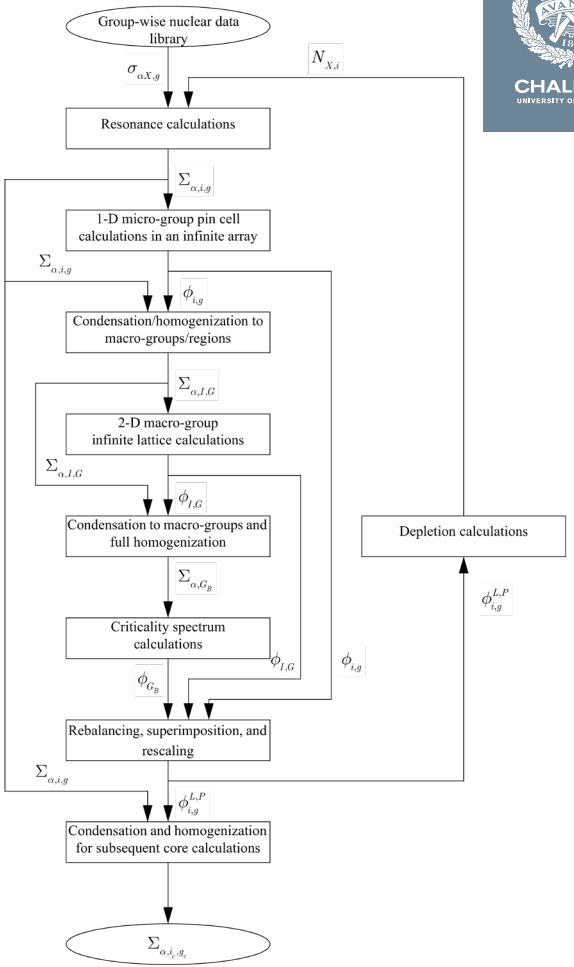
  Entire procedure **repeated** for different sets of **local conditions** that cannot be determined for the subsystem:
  - **History** effects (burnup b inclusive)
  - **Instantaneous** effects

  ➢Macroscopic cross-sections then "**functionalized**" as:

$$\Sigma_{\alpha,g}\left(\mathbf{r},t\right) \equiv \Sigma_{\alpha,g}\left[b\left(\mathbf{r},t\right), HE1\left(\mathbf{r},t\right), HE2\left(\mathbf{r},t\right), \ldots, IE1\left(\mathbf{r},t\right), IE2\left(\mathbf{r},t\right), \ldots\right]$$

Macroscopic cross-section generation in neutronics

- “**Multi-scale**” approach followed:



Closing the coarse mesh thermal-hydraulic equations

- Need to have "**consistent**" quantities appearing in all balance equations:
  - $\left\langle \underline{\alpha_k} \underline{\underline{c_k}} \right\rangle$ replaced with $\left\langle \underline{\alpha_k} \right\rangle \underline{\underline{\widehat{c_k}}}$ by defining proper averaging operator:

$$\underline{\underline{\widehat{c_k}}} = \frac{\frac{1}{V}\int_V \underline{\alpha_k} \underline{\underline{c_k}} d^3\mathbf{r}}{\frac{1}{V}\int_V \underline{\alpha_k} d^3\mathbf{r}}$$

  - $\left\langle \underline{\alpha_k} \underline{\underline{\left(\rho_k d_k\right)}} \right\rangle$ replaced with $\left\langle \underline{\alpha_k} \right\rangle \underline{\underline{\widehat{\rho_k}}}\,\underline{\underline{\widehat{d_k}}}$ by defining proper averaging operator:

$$\underline{\underline{\widehat{d_k}}} = \frac{\frac{1}{V}\int_V \underline{\alpha_k} \underline{\underline{\left(\rho_k d_k\right)}} d^3\mathbf{r}}{\frac{1}{V}\int_V \underline{\alpha_k} \underline{\underline{\rho_k}} d^3\mathbf{r}}$$

Closing the coarse mesh thermal-hydraulic equations

- The previous transformation also introduces **new cross-terms**: $\widehat{\underline{\underline{\left(\mathbf{v}_k \otimes \mathbf{v}_k\right)}}}$, $\widehat{\underline{\underline{\left(e_k \mathbf{v}_k\right)}}}$, $\widehat{\underline{\underline{\left(\boldsymbol{\tau}_k \cdot \mathbf{v}_k\right)}}}$ and $\widehat{\underline{\underline{\left(P_k \mathbf{v}_k\right)}}}$
  - Terms handled by assuming that:

$$c_k = \underline{\underline{c_k}} + c_k{}' \qquad \text{with} \qquad \underline{\underline{c_k}}{}' = 0$$

  - Introducing some other approximations (not detailed here), one obtains:

$$\widehat{\underline{\underline{\left(\mathbf{v}_k \otimes \mathbf{v}_k\right)}}} \approx \left(\widehat{\underline{\underline{\mathbf{v}_k}}} \otimes \widehat{\underline{\underline{\mathbf{v}_k}}}\right) + \frac{\left\langle \underline{\alpha_k} \underline{\underline{\rho_k}} \underline{\underline{\left(\mathbf{v}_k{}' \otimes \mathbf{v}_k{}'\right)}} \right\rangle}{\left\langle \underline{\alpha_k} \right\rangle \widehat{\underline{\underline{\rho_k}}}}$$

$$\widehat{\underline{\underline{\left(e_k \mathbf{v}_k\right)}}} \approx \widehat{\underline{\underline{e_k}}}\,\widehat{\underline{\underline{\mathbf{v}_k}}} + \frac{\left\langle \underline{\alpha_k} \underline{\underline{\rho_k}} \underline{\underline{\left(e_k{}' \mathbf{v}_k{}'\right)}} \right\rangle}{\left\langle \underline{\alpha_k} \right\rangle \widehat{\underline{\underline{\rho_k}}}}$$

turbulent terms

$$\widehat{\underline{\underline{\left(\boldsymbol{\tau}_k \cdot \mathbf{v}_k\right)}}} \approx \widehat{\underline{\underline{\boldsymbol{\tau}_k}}} \cdot \widehat{\underline{\underline{\mathbf{v}_k}}}$$

$$\widehat{\underline{\underline{\left(P_k \mathbf{v}_k\right)}}} \approx \widehat{\underline{\underline{P_k}}}\,\widehat{\underline{\underline{\mathbf{v}_k}}}$$

Closing the coarse mesh thermal-hydraulic equations

- When looking at the resulting equations:

Too many unknown variables compared to the **number of available equations**

➢Need to **close the system of equations** by introducing **empirically-derived closure laws**, e.g.:

- For the terms related to **transfers** at the liquid/vapor interfaces
- For the terms related to **transfers** between **each of the two phases**, respectively, and the **solid walls**
- For the **turbulent terms**

and by **relating** some **phasic quantities** to each other, e.g.

- **Temperature**
- **Pressure**

Resolving the multi-physics interdependencies

Resolving the multi-physics interdependencies

- Modelling of nuclear systems has typically been made focusing on **one physics at a time** (with frozen boundary conditions from the other physics)
- "**Less conservative**" estimates rely on **more faithful coupling strategies** where the **various physics are equally well described**

Resolving the multi-physics interdependencies

- Multi-physics problem generically written as (before time discretization):

$$\frac{d\mathbf{u}}{dt}\left(t\right) = \mathbf{F}\left(\mathbf{u}, t\right)$$

- In case of two physics φ_1 and φ_2, problem solved as:

$$\frac{d\mathbf{u}}{dt}\left(t\right) = \mathbf{F}\left(\mathbf{u}, t\right)$$

monolithic approach

Resolving the multi-physics interdependencies

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$$\frac{d\mathbf{u}}{dt}\left(t\right) = \mathbf{F}\left(\mathbf{u}, t\right)$$

- In case of two physics φ_1 and φ_2, problem solved as:

$$\frac{d}{dt}\begin{bmatrix}\mathbf{u}_{\varphi_1}\left(t\right)\\ \mathbf{u}_{\varphi_2}\left(t\right)\end{bmatrix} = \mathbf{F}\left(\begin{bmatrix}\mathbf{u}_{\varphi_1}\left(t\right)\\ \mathbf{u}_{\varphi_2}\left(t\right)\end{bmatrix}, t\right)$$

or

$$\frac{d}{dt}\begin{bmatrix}\mathbf{u}_{\varphi_1}\left(t\right)\\ \mathbf{u}_{\varphi_2}\left(t\right)\end{bmatrix} = \begin{bmatrix}\mathbf{F}_{\varphi_1}\left(\begin{bmatrix}\mathbf{u}_{\varphi_1}\left(t\right)\\ \mathbf{u}_{\varphi_2}\left(t\right)\end{bmatrix}, t\right)\\ \mathbf{F}_{\varphi_2}\left(\begin{bmatrix}\mathbf{u}_{\varphi_1}\left(t\right)\\ \mathbf{u}_{\varphi_2}\left(t\right)\end{bmatrix}, t\right)\end{bmatrix}$$

monolithic approach

segregated approach

Resolving the multi-physics interdependencies

- **Segregated approaches mostly used** because of the extensive verification and validation of mono-physics solvers
- **Different ways** to implement **segregated approaches**:
  - **Exchange of data** via **input/output files** (+ **scripts**)
  - **Exchange of data** within the **computer memory**
    - Mono-physics solvers **compiled into one executable**
    - Use of a **message passing interface**

- Remark: using one single software can still rely on segregated approaches

Resolving the multi-physics interdependencies

- Multi-physics problem rewritten as:

$$\frac{d}{dt}\begin{bmatrix}\mathbf{u}_{\varphi_1}(t)\\ \mathbf{u}_{\varphi_2}(t)\end{bmatrix}=\begin{bmatrix}\mathbf{L}_{\varphi_1}(t) & 0\\ 0 & \mathbf{L}_{\varphi_2}(t)\end{bmatrix}\times\begin{bmatrix}\mathbf{u}_{\varphi_1}(t)\\ \mathbf{u}_{\varphi_2}(t)\end{bmatrix}+\quad\ldots$$

where dependence on the other physics assumed to be in the non-linearities

Resolving the multi-physics interdependencies

- Multi-physics problem rewritten as:

$$\frac{d}{dt}\begin{bmatrix}\mathbf{u}_{\varphi_1}(t)\\ \mathbf{u}_{\varphi_2}(t)\end{bmatrix}=\begin{bmatrix}\mathbf{L}_{\varphi_1}(t) & 0\\ 0 & \mathbf{L}_{\varphi_2}(t)\end{bmatrix}\times\begin{bmatrix}\mathbf{u}_{\varphi_1}(t)\\ \mathbf{u}_{\varphi_2}(t)\end{bmatrix}+\begin{bmatrix}\mathbf{N}_{\varphi_1}\left(\begin{bmatrix}\mathbf{u}_{\varphi_1}(t)\\ \mathbf{u}_{\varphi_2}(t)\end{bmatrix},t\right)\\ \\ \\ \end{bmatrix}$$

where dependence on the other physics assumed to be in the non-linearities

Resolving the multi-physics interdependencies

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where dependence on the other physics assumed to be in the non-linearities

Resolving the multi-physics interdependencies

- **Segregated** or **operator splitting** strategies:
  use of each of the mono-physics solvers in their non-altered forms and on some exchange of information/data between the solvers

➢Three basic approaches:

- Non-linearities from the other mono-physics solver evaluated at the previous time step

$$\mathbf{N}_{\varphi_k}\left(\begin{bmatrix}\mathbf{u}_{\varphi_k}\left(t+\Delta t\right)\\ \mathbf{u}_{\varphi_{l\neq k}}\left(t+\Delta t\right)\end{bmatrix}, t+\Delta t\right) \quad \text{replaced by} \quad \mathbf{N}_{\varphi_k}\left(\begin{bmatrix}\mathbf{u}_{\varphi_k}\left(t+\Delta t\right)\\ \mathbf{u}_{\varphi_{l\neq k}}\left(t\right)\end{bmatrix}, t+\Delta t\right)$$

➢**Non-linear inconsistencies** introduced

Resolving the multi-physics interdependencies

- **Segregated** or **operator splitting** strategies:
  use of each of the mono-physics solvers in their non-altered forms and on some exchange of information/data between the solvers

➢Three basic approaches:

- φ_1 first solved using the non-linearities from the other mono-physics solver φ_2 evaluated at the previous time step

$$\mathbf{N}_{\varphi_1}\left(\begin{bmatrix}\mathbf{u}_{\varphi_1}(t+\Delta t)\\ \mathbf{u}_{\varphi_2}(t+\Delta t)\end{bmatrix}, t+\Delta t\right) \text{ replaced by } \mathbf{N}_{\varphi_1}\left(\begin{bmatrix}\mathbf{u}_{\varphi_1}(t+\Delta t)\\ \mathbf{u}_{\varphi_2}(t)\end{bmatrix}, t+\Delta t\right)$$

φ_2 then solved using the solution $\mathbf{u}^*_{\varphi_1}(t+\Delta t)$ evaluated above at the current time step

$$\mathbf{N}_{\varphi_2}\left(\begin{bmatrix}\mathbf{u}_{\varphi_1}(t+\Delta t)\\ \mathbf{u}_{\varphi_2}(t+\Delta t)\end{bmatrix}, t+\Delta t\right) \text{ replaced by } \mathbf{N}_{\varphi_2}\left(\begin{bmatrix}\mathbf{u}^*_{\varphi_1}(t+\Delta t)\\ \mathbf{u}_{\varphi_2}(t+\Delta t)\end{bmatrix}, t+\Delta t\right)$$

➢**Non-linear inconsistencies** introduced

Resolving the multi-physics interdependencies

- **Segregated** or **operator splitting** strategies:
  use of each of the mono-physics solvers in their non-altered forms and on some exchange of information/data between the solvers

➢Three basic approaches:

- **Successive updates** of the solution vector as:

$$\begin{bmatrix} \mathbf{u}^1_{\varphi_1}\left(t+\Delta t\right) \\ \mathbf{u}_{\varphi_2}\left(t\right) \end{bmatrix}$$

Resolving the multi-physics interdependencies

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- **Successive updates** of the solution vector as:

$$\begin{bmatrix} \mathbf{u}^1_{\varphi_1}\left(t+\Delta t\right) \\ \mathbf{u}_{\varphi_2}\left(t\right) \end{bmatrix} \rightarrow \begin{bmatrix} \mathbf{u}^1_{\varphi_1}\left(t+\Delta t\right) \\ \mathbf{u}^1_{\varphi_2}\left(t+\Delta t\right) \end{bmatrix}$$

Resolving the multi-physics interdependencies

- Segregated or operator splitting strategies:
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Resolving the multi-physics interdependencies

- Segregated or operator splitting strategies:
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Resolving the multi-physics interdependencies

- Segregated or operator splitting strategies:
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➢Three basic approaches:

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  ➢**Non-linear inconsistencies resolved**

  ➢**Convergence** usually slow/difficult

Resolving the multi-physics interdependencies

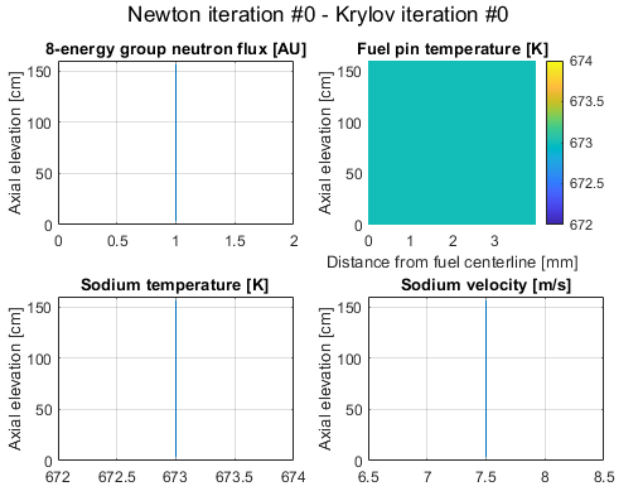
- **Monolithic** approaches:
  Entire multi-physics problem rewritten as "**one**" problem:

$$\mathbf{H}\left(\mathbf{u}\left(t+\Delta t\right)\right)=\mathbf{0}$$

➢ Due to the different time scales and characteristic lengths of each physics, the problem is often **ill-conditioned**: need to **pre-condition** the problem

Resolving the multi-physics interdependencies

- Example of a **1-dimensional heterogeneous model** of a **sodium-cooled fast reactor** in **steady-state conditions**:



Integrated approach (Jacobian Free Newton Krylov method)

Resolving the multi-physics interdependencies

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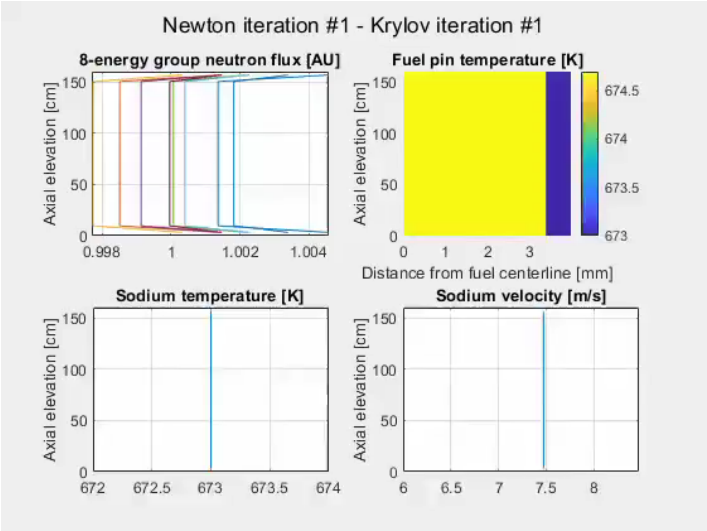


Integrated approach (Jacobian Free Newton Krylov method)

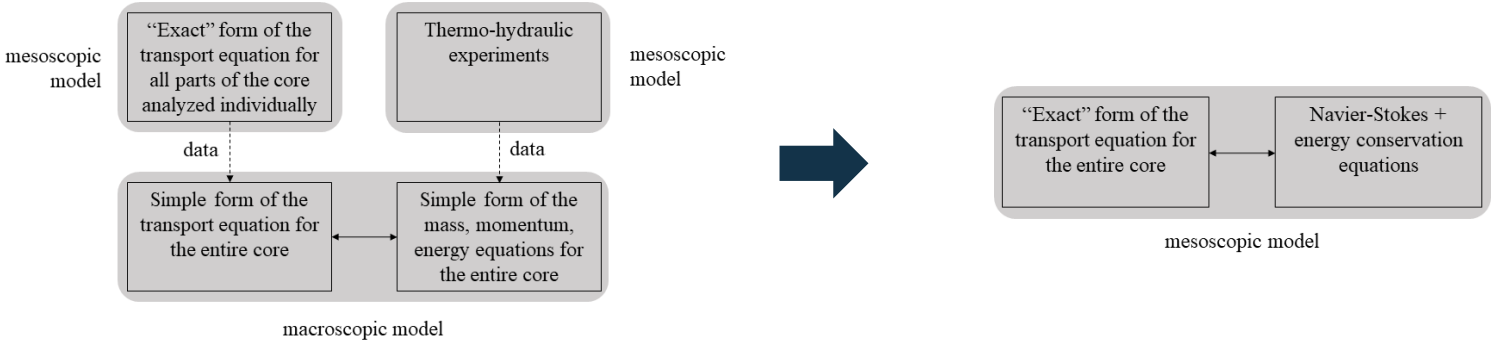
Conclusions and outlook

Conclusions and outlook

- **“Multi-scale”** approach followed:
  - **Neutronics**: **subsystems solved** at various levels of refinement before **modelling the entire system**
  - **Thermal-hydraulics**: modelling of only the **large-scale phenomena** with the **small-scale** (and h**igh-frequency**) **phenomena** considered via **experimentally-derived correlations**
- **Multi-physics** coupling:
  - **Segregated** approaches:
    - **Pros**: Extensive V&V + codes tuned to a specific purpose
    - **Cons**: Reaching convergence might be challenging + codes tuned to a specific purpose
  - **Monolithic** approaches:
    - **Pros**: Better control of convergence
    - **Cons**: Robustness of the methods might be challenging

Conclusions and outlook

- On-going international efforts to **couple the physics** at the **small scales**:



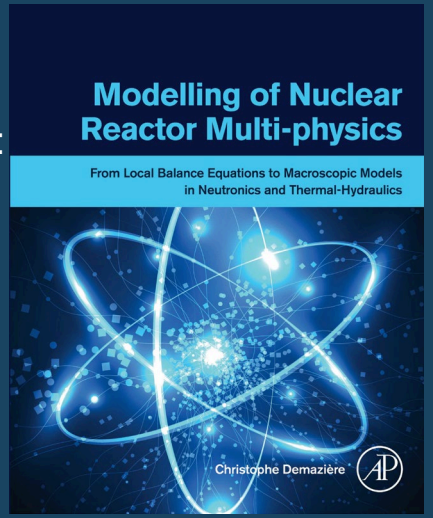
Deterministic modelling of nuclear systems

Spring School on Sodium Cooled Fast Reactors

University of Cambridge, March 29th-31st, 2021 – online

Prof. Christophe Demazière
demaz@chalmers.se

Learn more about reactor modelling:
(Elsevier/Academic Press book)



DREAM

TASK FORCE ON
DETERMINISTIC REACTOR MODELLING