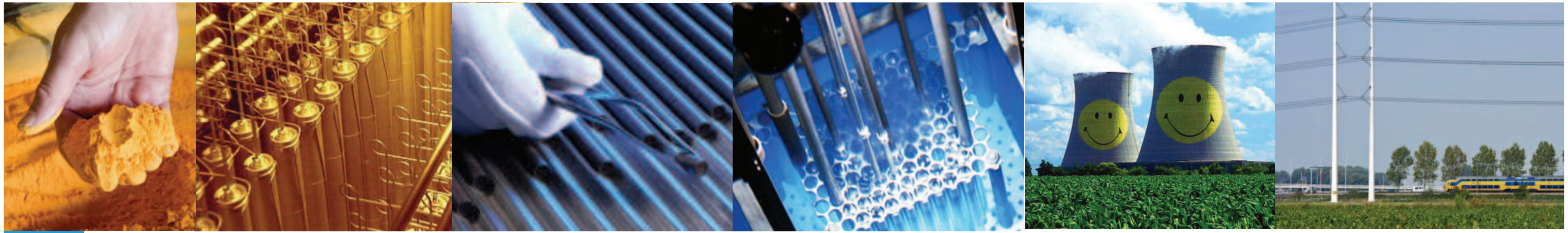


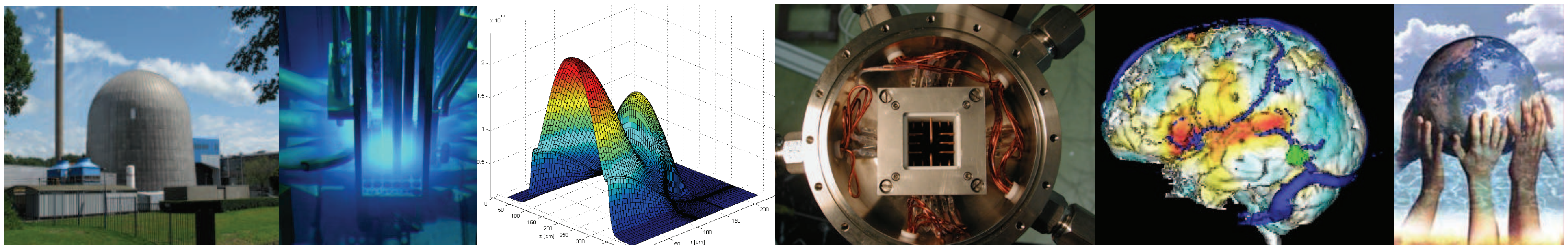
Multi-Physics Simulation of Molten Salt Reactors

Danny Lathouwers

Delft University of Technology

Dept. of Radiation Science and Technology

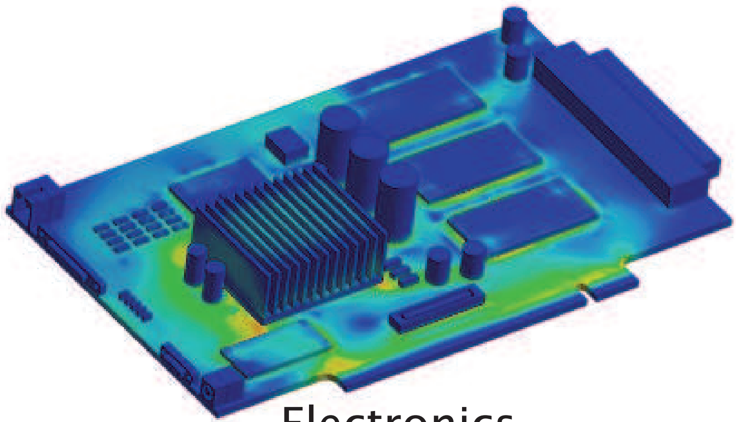
Co-workers: Michiel Hoogmoed, Jan Leen Kloosterman, Dion Koeze, Carlo Fiorina, Lodewijk Frima, Joseph Kophazi, Erik van der Linden, Marco Tiberga, …



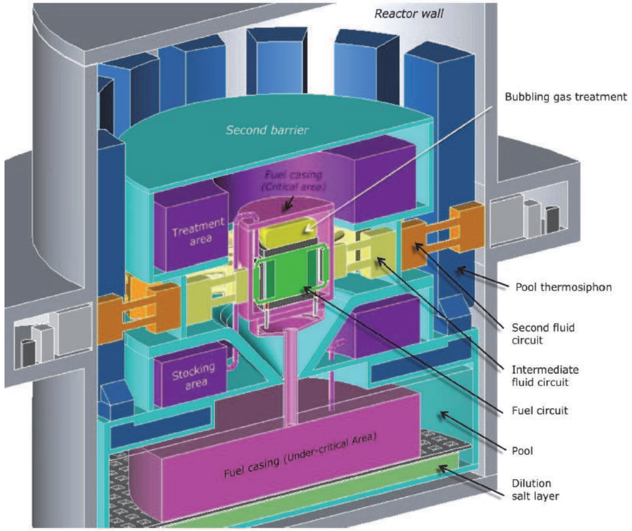
Multiphysics in various fields

Fluid-structure interaction

Furnace (thermal, chemistry)



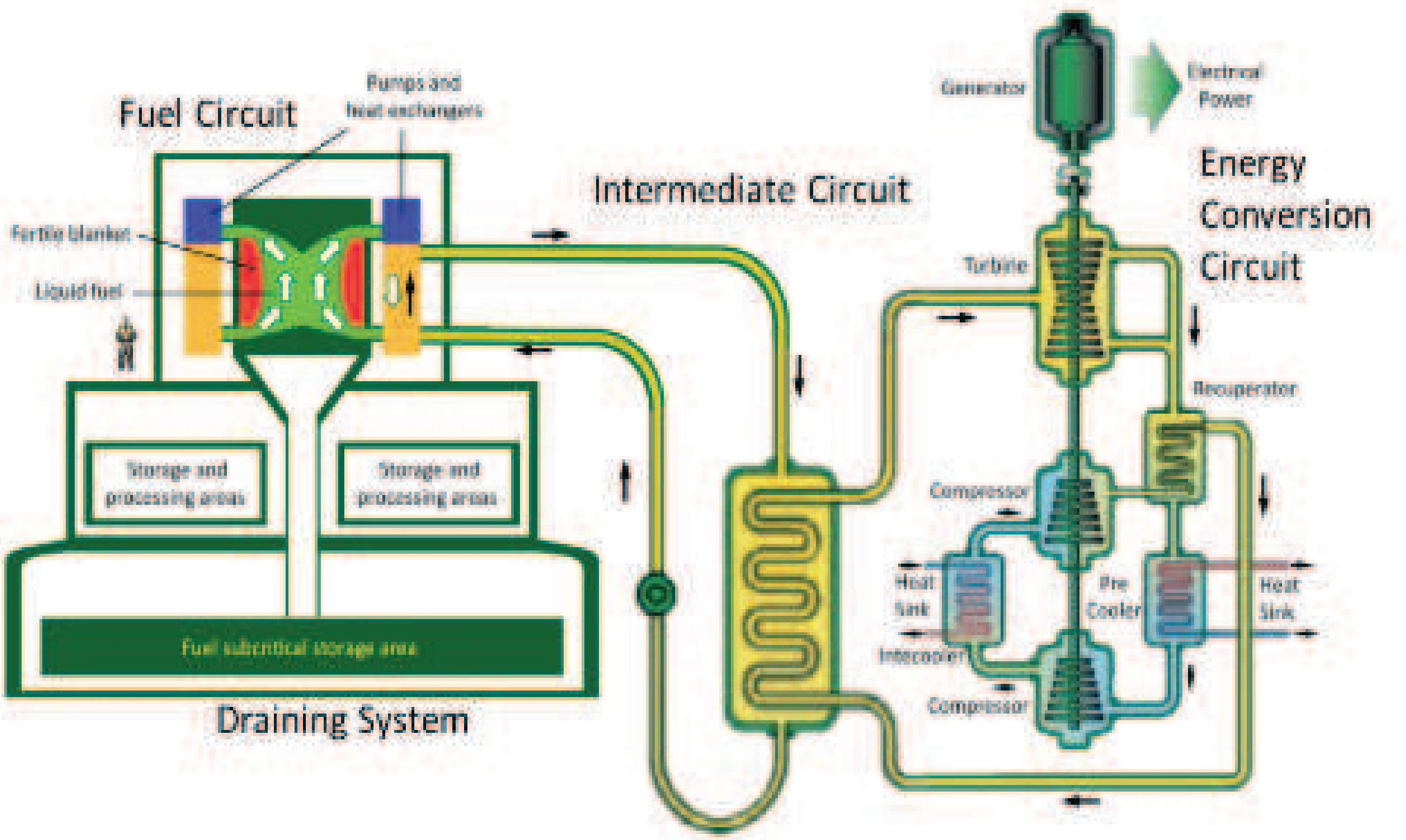
Electronics
(thermal, stress analysis)



Nuclear (flow, thermal,
stress, radiation)

SAMOFAR

MSFR



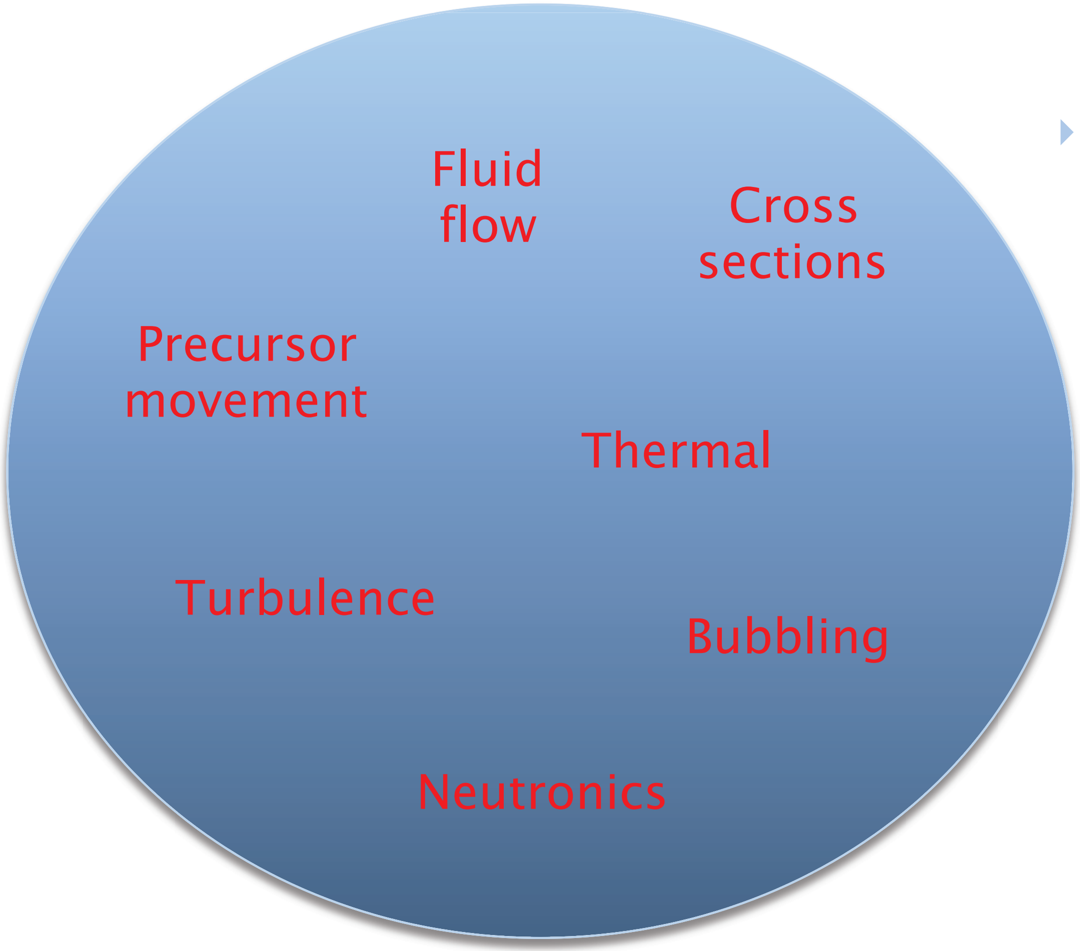
Fuel Circuit
Pumps and heat exchangers
Fertile blanket
Liquid fuel
Storage and processing areas
Storage and processing areas
Fuel subcritical storage area
Draining System
Intermediate Circuit
Generator
Electrical Power
Energy Conversion Circuit
Turbine
Recuperator
Compressor
Heat Sink
Pre Cooler
Heat Sink
Intercooler
Compressor

Main topics discussed

- Physics involved: time-scales, complexity
- Coupling strategies (pro/cons)
- MSRE application
- MSFR application
- Concluding remarks

SAMOFAR

Multiphysics in the MS(F)R

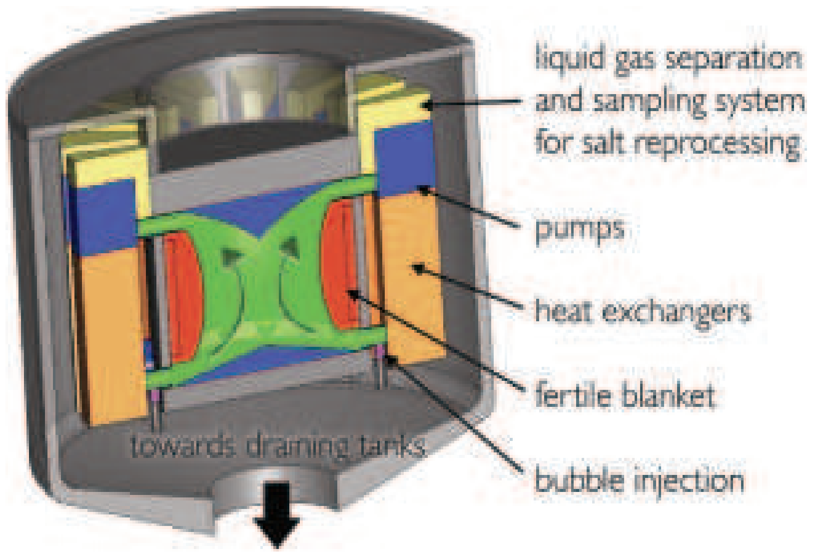


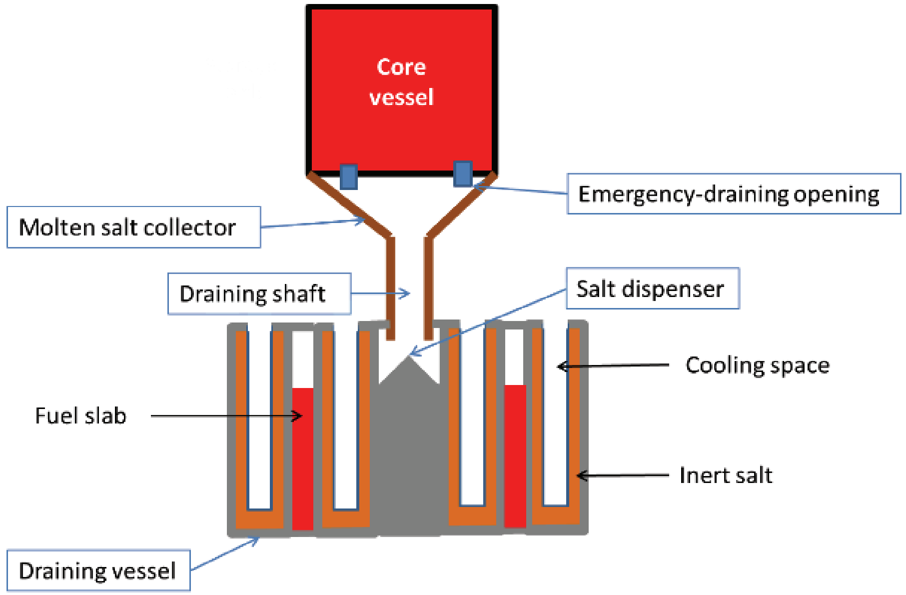
- Capabilities needed
  - Moving fuel -> moving precursors
  - Complex geometry
  - Three-dimensionality
  - Heat transfer, (two-phase) fluid flow, stress analysis, neutronics
  - Temperature feedback effects on cross sections
  - Voidage feedback from bubbling and on effect flow structure

SAMOFAR

Relevant transients

- Two types of transients are considered
  - Fuel circuit transients
  - Transients involving the emergency draining tank





SAMOFAR

- Main transients chosen

Code	Class	Transient	Initiating event / description
1.1.a	1 – Fuel Circuit	ULOHS	a) Reduction of the mass flow rate in the intermediate circuit
1.2.a	1 – Fuel Circuit	ULOFF	a) Fuel circuit pump failure
1.3.	1 – Fuel Circuit	TLOP	Phase 0 and phase 2
1.4.a	1 – Fuel Circuit	OVC	a) Increase in the fuel salt flow
1.4.c		OVC	c) Decrease of temperature in the intermediate circuit
1.6.a	1 – Fuel Circuit	RAA	a) Increase/decrease of salt (fissile) volume in the core cavity or heterogeneity of fissile salt (positive/negative reactivity insertion)
2.1.a	2 – EDS	EDS-LOHS	a) Insufficient cooling circuit flow
2.3	2 – EDS	EDS-BA	Blockage of fuel salt

Neutronics Modeling

Consider full transport model as example

$$\frac{1}{v}\frac{\partial \varphi_g}{\partial t} + \widehat{\Omega}\cdot\nabla\varphi_g + \Sigma_{t,g}\varphi_g = \sum_{g'}\int_{4\pi}\Sigma_{s,g'\to g}(\widehat{\Omega}'\to\widehat{\Omega})\varphi_{g'}d\widehat{\Omega}' + \frac{\chi_g}{4\pi k_{eff}}(1-\beta)\sum_g \nu\Sigma_{f,g}\int_{4\pi}\varphi_g d\widehat{\Omega} + \sum_i \lambda_i C_i$$

$$\frac{\partial C_i}{\partial t} + \lambda_i C_i + \boxed{\nabla\cdot\vec{u}C_i} = \beta_i\sum_g \nu\Sigma_{f,g}\int_{4\pi}\varphi_g d\widehat{\Omega}$$

Magnitude of the problem

- Mesh: 10000 elements
- Angle: 24 in practice for MSR
- 8 precursors
- Space: Linear polynomials ->4 basis functions
- Energy: pm 10 groups

→ No dof: pm 10 Million (+ time stepping)

Diffusion is a (much) cheaper alternative

SAMOFAR

Neutronics time scales

Time scales relevant to the neutronics part of the problem

- Prompt time scale $\tau = \frac{\Lambda}{\beta - \rho} < 1ms$
- Reactor period $\tau = \frac{1}{\rho}\sum_i \frac{\beta_i}{\lambda_i} >> 1s$

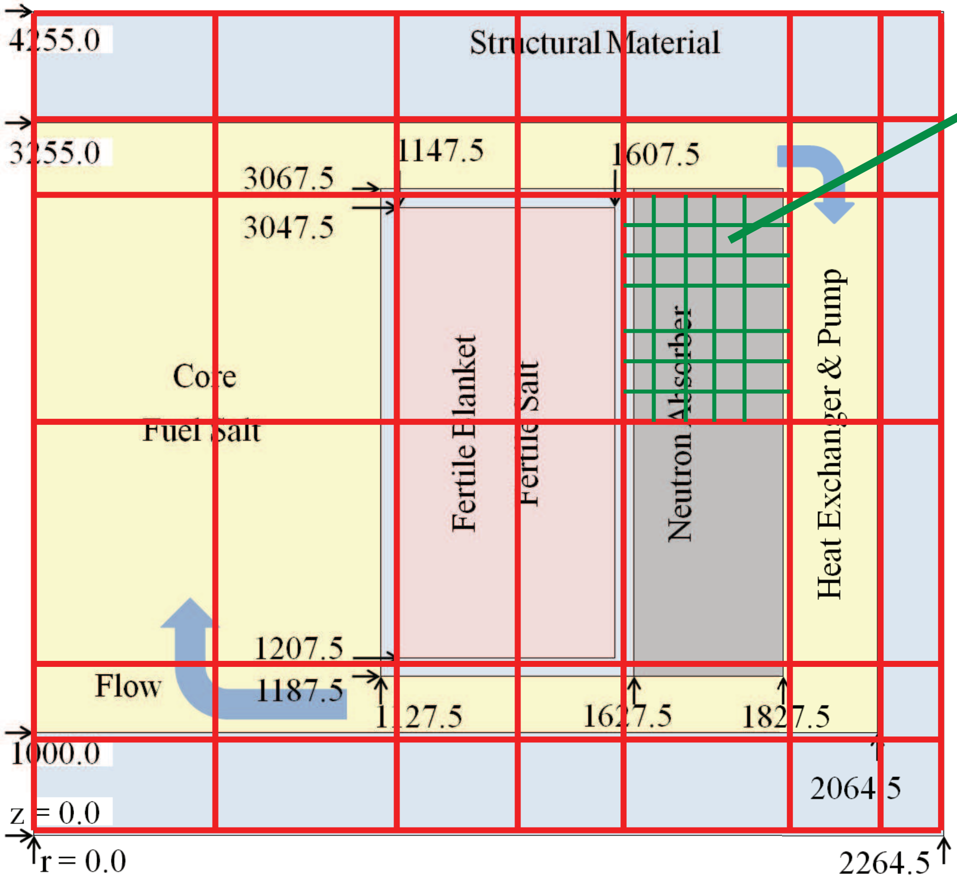
Wide range of time scales

- Usually no need to resolve prompt time scale
- Most neutronics codes are implicit in time (or use Prompt Jump Approximation)

Cross section processing

- Cross sections depend on space and time through temperature and composition
- Mapping needed of the system select proper xs set (in practice 20-1000 sets are used)
- Each mesh element corresponds to specific material
- Libraries need to be generated (Scale, Serpent, etc). Around 10 groups sufficient for MSFR
- XS need to be interpolated wrt temperature (either for each cell or for each material region using an average T)
- Density dependence as well (bubbling)
- XS generation somewhat of an art

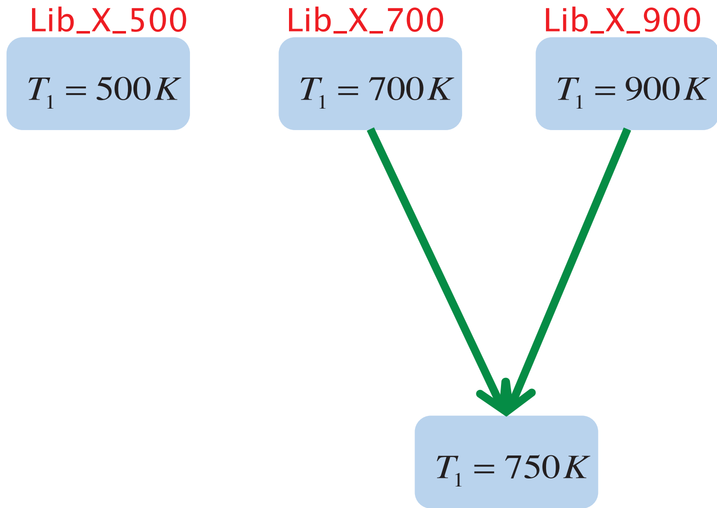
Cross section mapping and interpolation



Segmentation of the domain

Element associated with region X, having temperature T=750K

Interpolate XS files for region X



$$\Sigma_i = \frac{\rho}{\rho_{ref}}\left(\Sigma_{i,ref} + A_i \log\frac{T}{T_{ref}}\right)$$

SAMOFAR

Flow Modeling

MSFR: turbulent flow
Boussinesq approximation reasonable in most cases

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot \rho \vec{u}\vec{u} = -\nabla p + \nabla \cdot \bar{\bar{\tau}}_{eff} - \rho \vec{g}\beta(T - T_{ref}) + S_u$$

$$\nabla \cdot \vec{u} = 0$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot \rho \vec{u} h = \nabla \cdot \lambda_{eff} \nabla T + P$$

$$+\text{Turbulence model}$$

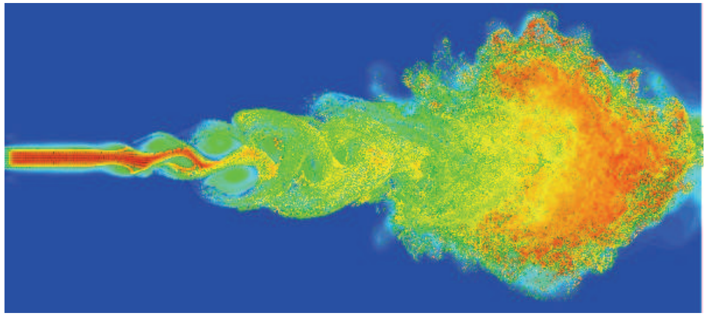
Magnitude of the problem

- Mesh: 40000 elements
- Space: Linear polynomials ->4 basis functions
- 5 main flow variables + turbulence model
- No dof: pm 1 Million (+ time stepping)

Fluid flow time scales

We deal with a turbulent flow with a large variety of spatial and time scales

- Large eddy turnover $\tau = \frac{L}{u} \sim 10s$
- Cascading (decay) $\tau = \frac{k}{\varepsilon} < 1s$
- Kolmogorov time scale $\tau = \left(\frac{\nu}{\varepsilon}\right)^{1/2} << 1s$



- We use RANS models where we do not resolve the small scale turbulence
- For stability reasons, turbulence production/dissipation terms usually handled implicitly

SAMOFAR

Data exchange

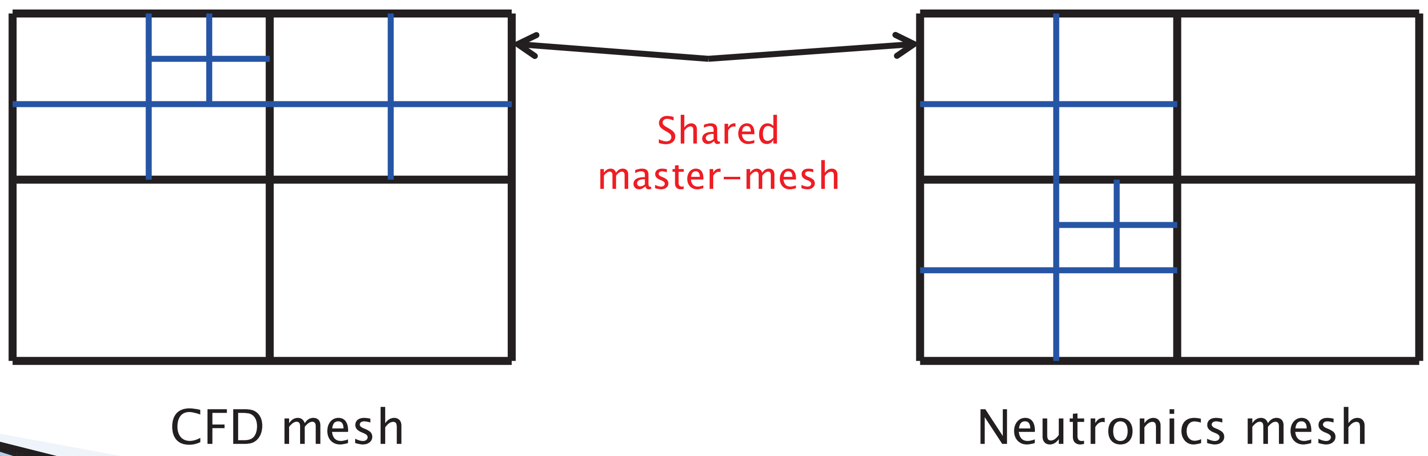
Meshes for each physics module not the same

=> interpolation required

Important properties:

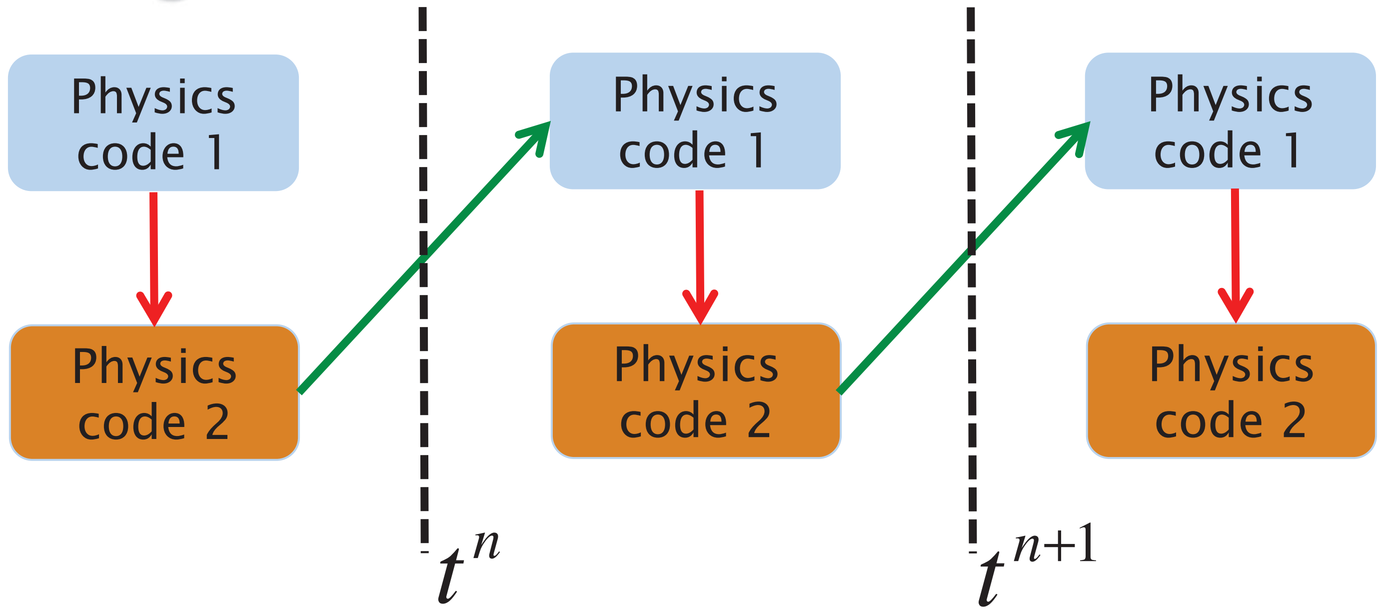
- Conservation
- Speed of interpolation

Hierarchic meshes combined with *Galerkin projection* satisfy both these properties.



SAMOFAR

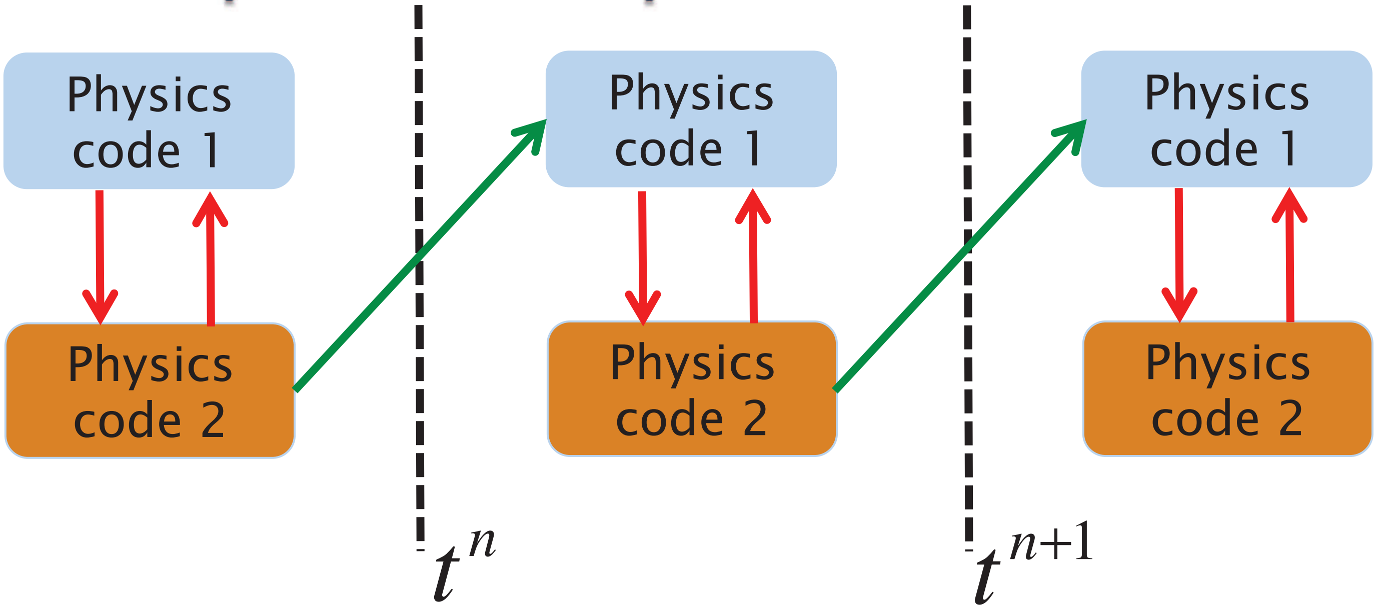
Conventional (loose) coupling
Splitting schemes



- Easy to implement using existing (black-box) codes
- Cheap on a time step basis
- At most first-order time accuracy
- Stability may be issue; though difficult to analyse
- Times at which to data needs exchange depends on physics and time scales

Tight coupling scheme

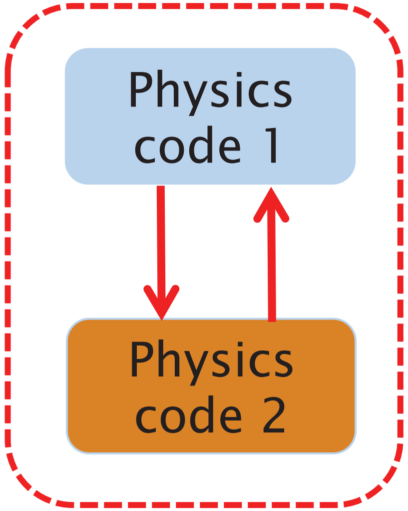
Iteration per time step



- Still easy to implement using existing codes
- Iteration may be expensive
- Time accuracy dictated by that of the individual codes (full potential can be achieved)
- Coupling no longer dominates stability

SAMOFAR

Towards improved efficiency



- *Sequential exchange of data* between codes is formally a Picard (fixed-point) iteration

$$u - f(u) = 0 \rightarrow u^{k+1} = f(u^k)$$

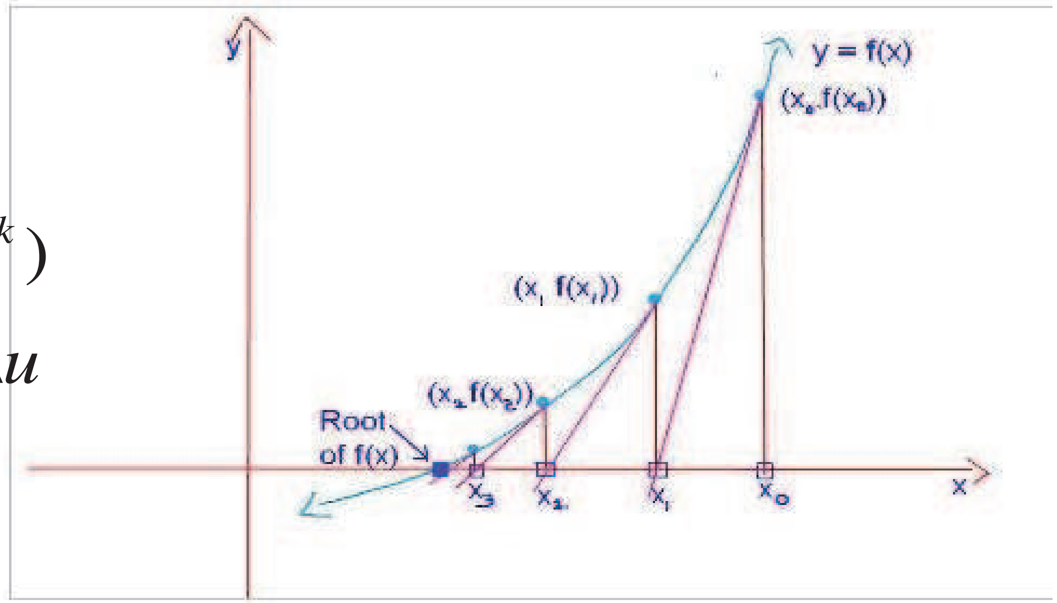
- Convergence in general is slow (linear)
- Easy to do (and often done!)

Variations

- Anderson acceleration: keeps a series of iterates and finds optimal combination
- Aitken acceleration: Keeps 3 iterates and combines to new
- ...

Newton's method

$$F(u)=0 \rightarrow \begin{cases} J\Delta u = -F(u^k) \\ u^{k+1} = u^k + \Delta u \end{cases}$$



- Quadratic convergence close to solution
- Requires *Jacobian* (intrusive!), mostly unavailable)
- Large linear system in each Newton iteration

Jacobian-Free Newton Krylov (JFNK)
(D. Knoll etc)

- Innovative idea combining:
  - Newton iteration for the non-linearity
  - Krylov method for the linear system in each step
  - A smart trick

- BUT: How possible without Jacobian?

- Krylov methods require matrix multiplication only: Jv

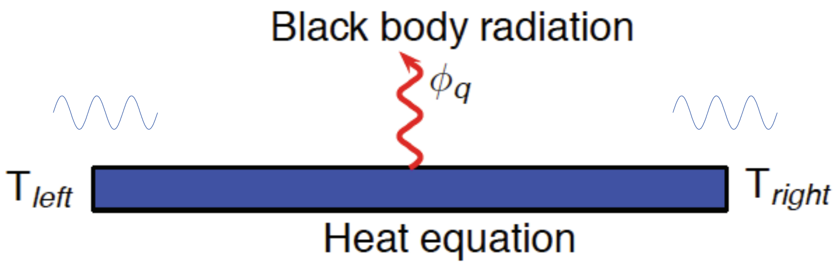
$$Jv \simeq \frac{F(u+\varepsilon v)-F(u)}{\varepsilon}$$

- JFNK only requires residual F

- Preconditioning for efficient Krylov is essential (usually Gauss-Seidel is used: physics preconditioning)

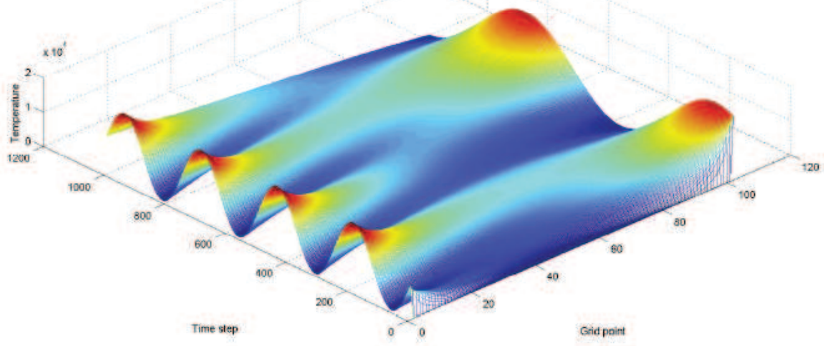
SAMOFAR

Coupling example: Toy problem

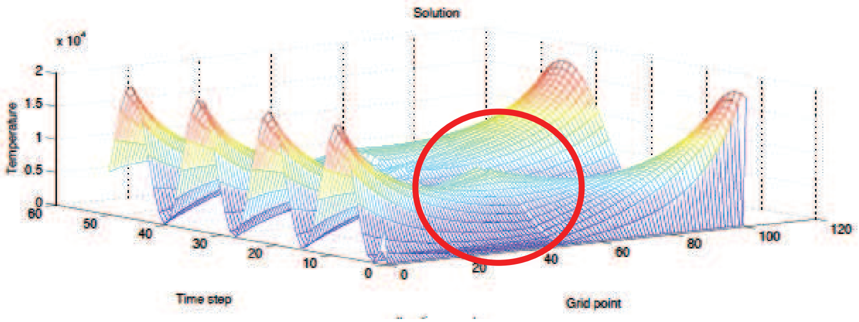


Physics 1: left half

Physics 2: right half

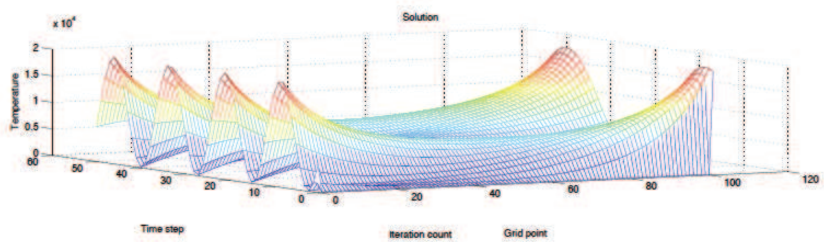


'Exact' solution



Traditional coupling

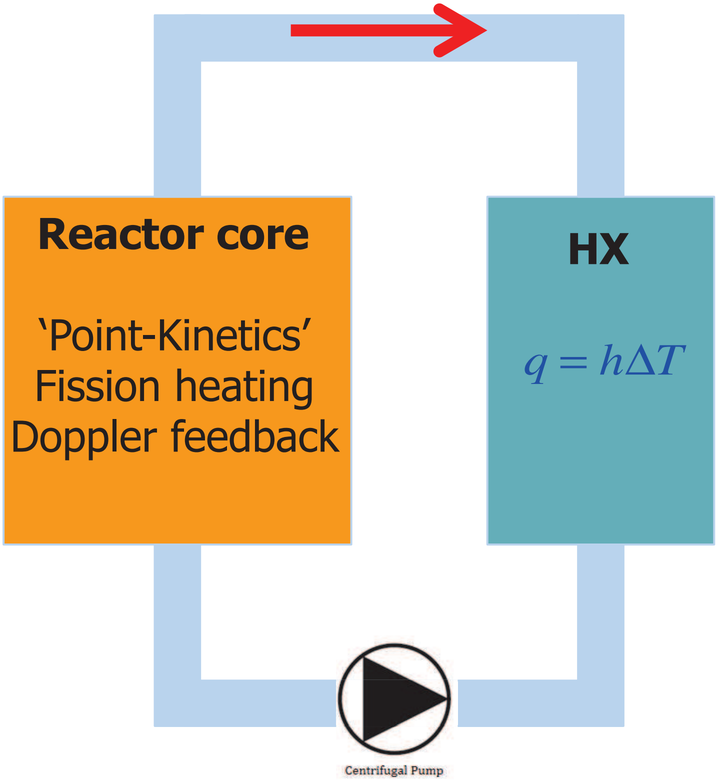
artifacts near coupling location



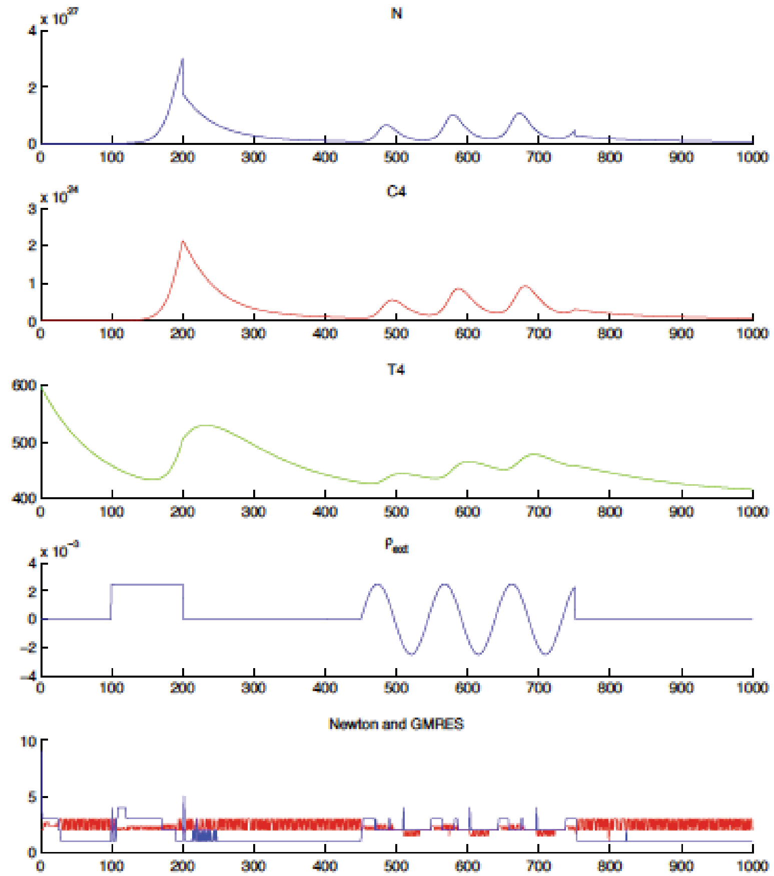
JFNK

Work of Dion Koeze (BSc thesis, 2009

Coupling example: MSR-loop



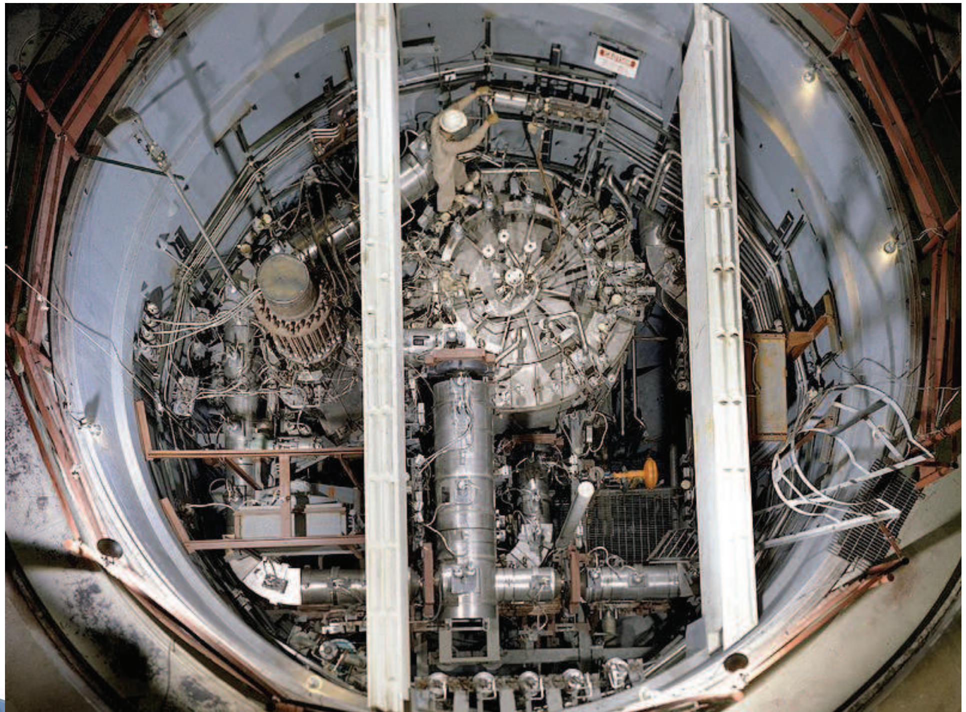
External reactivity transient



- JFNK stable and efficient
- Relatively easy problem (1-2 Newton steps)
- Some hick-ups when using large external reactivity with (too) large time-steps

SAMOFAR

Molten Salt Reactor Experiment



SAMOFAR

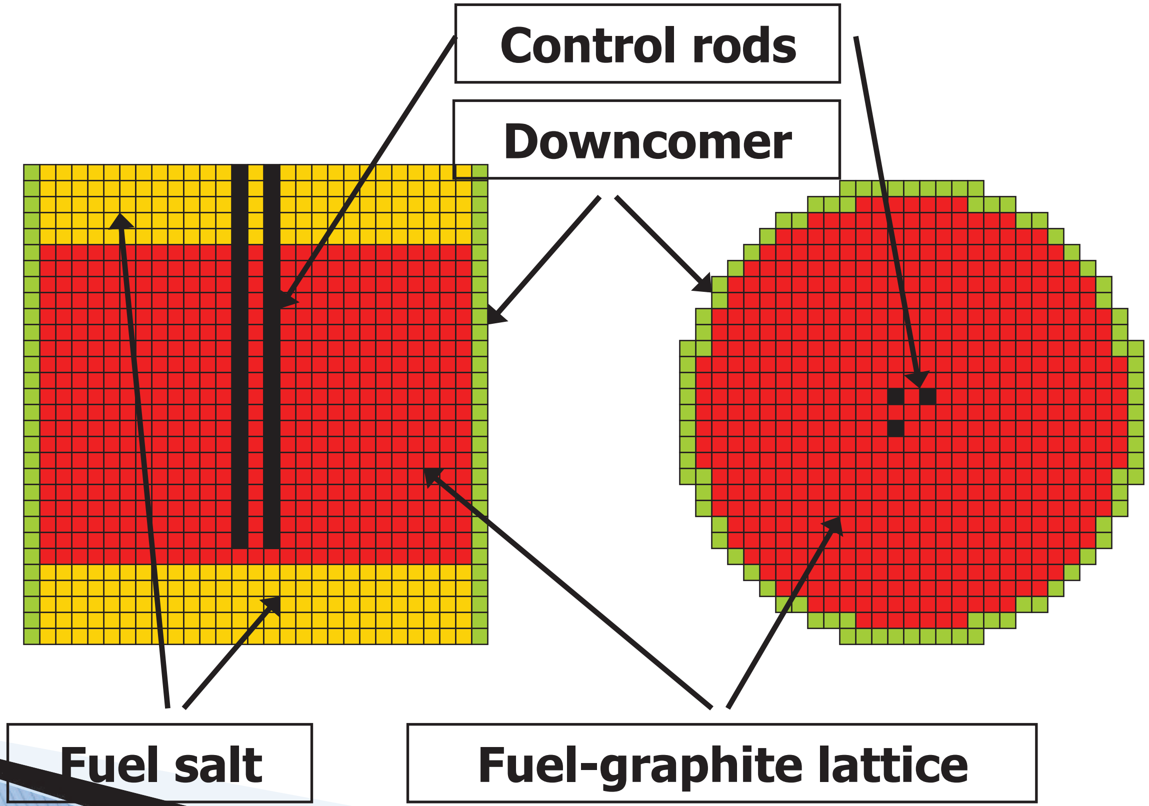
Molten Salt Reactor Experiment

- Developing calculation scheme for MSR
  - 3D
  - time-dependent
  - feedback by coupling neutronics and thermal calculations
  - Model the MSRE
  - Keep programs general

- Assumptions
  - Fuel velocity field is input
  - Flow parallel to the axis of the core

MSRE: 3D model

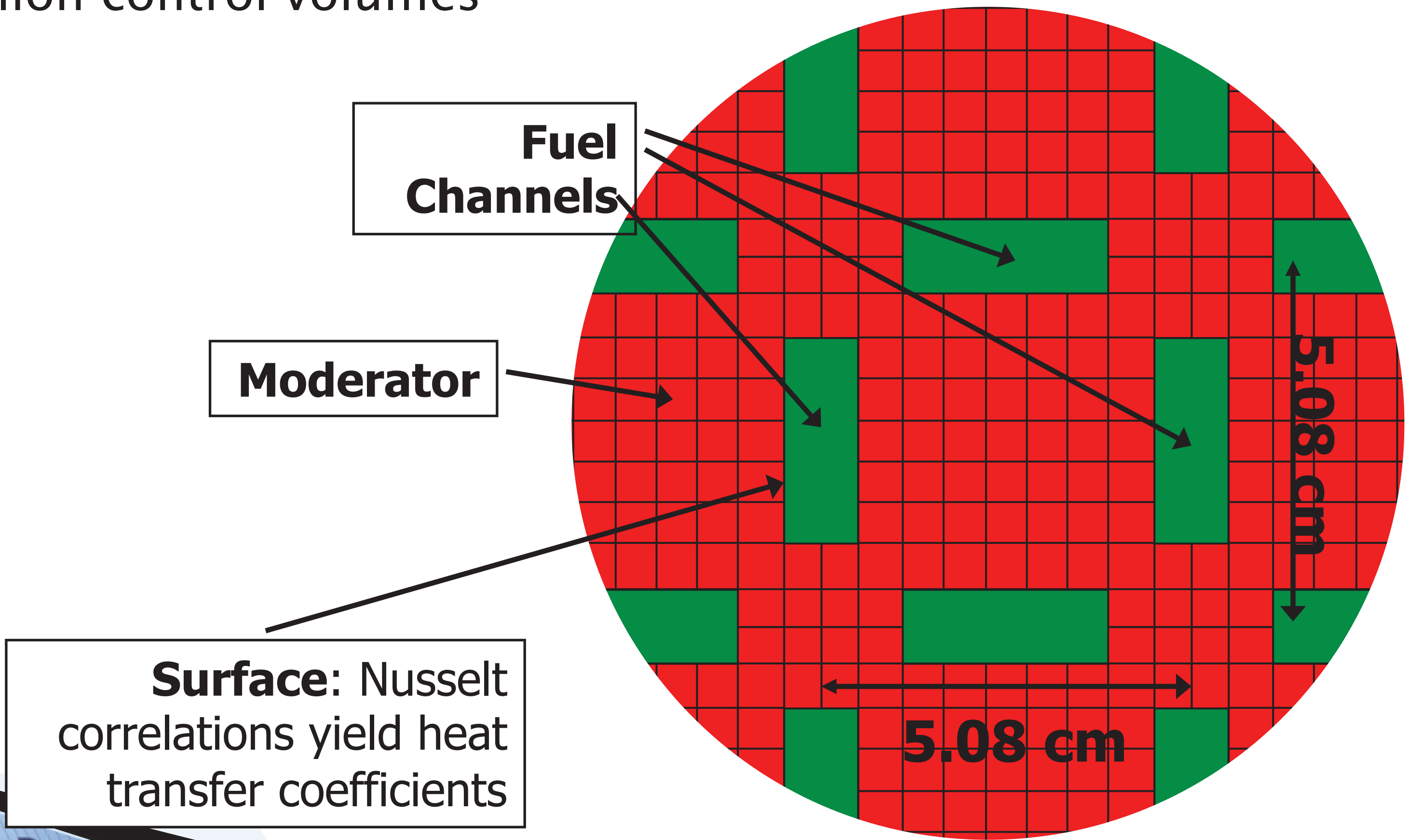
- Approximating cylindrical reactor in X-Y-Z geometry
- 8 group cross section library by SCALE
- Internal albedo boundaries for control rods



SAMOFAR

MSRE: 3D model

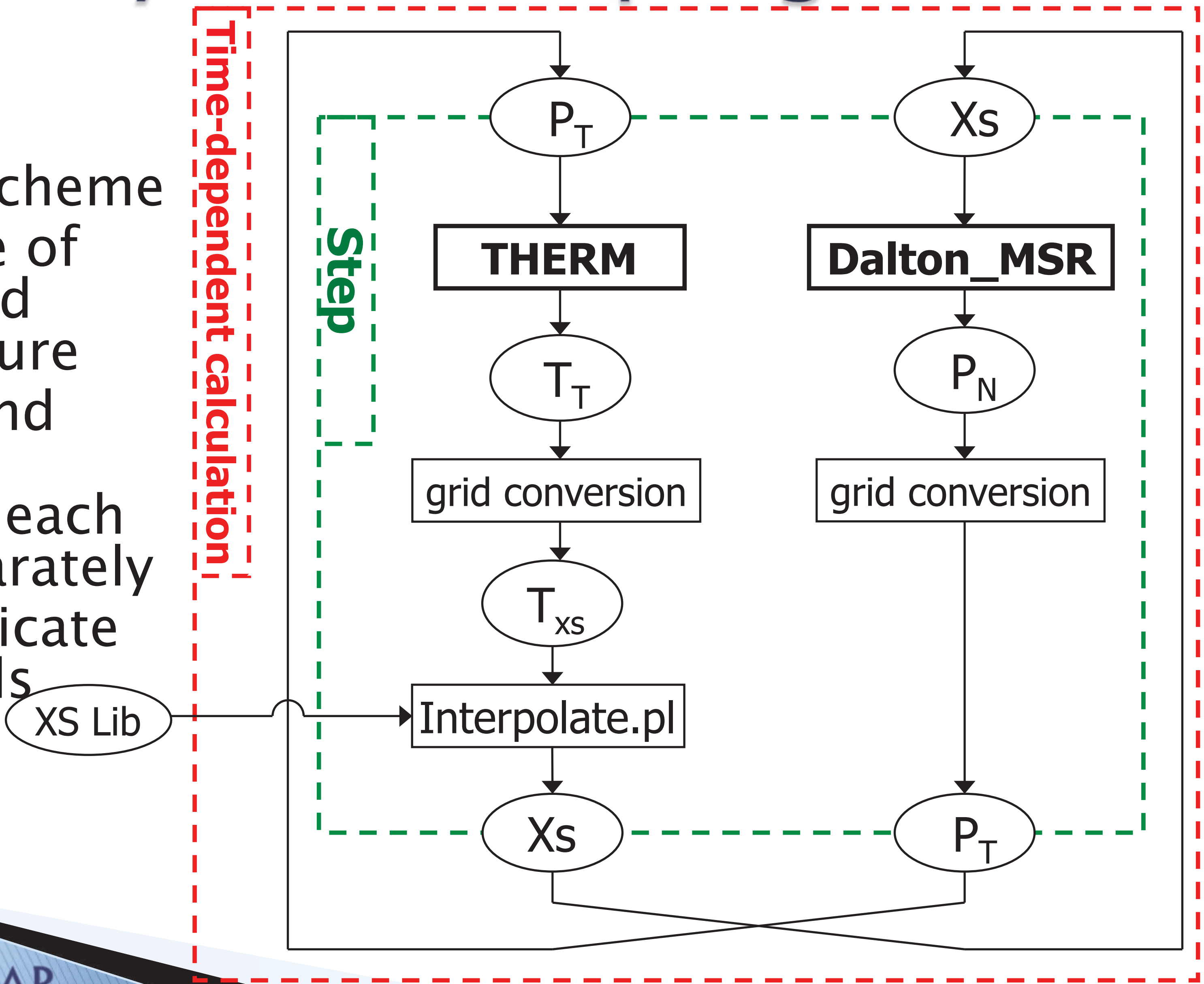
- Fuel: Heat convection (vertical)
- Moderator: Heat conduction (3D)
- Individually calculating each fuel channel (1150 channels)
- Bulk temperatures for fuel channels
- ~1.5 million control volumes



SAMOFAR

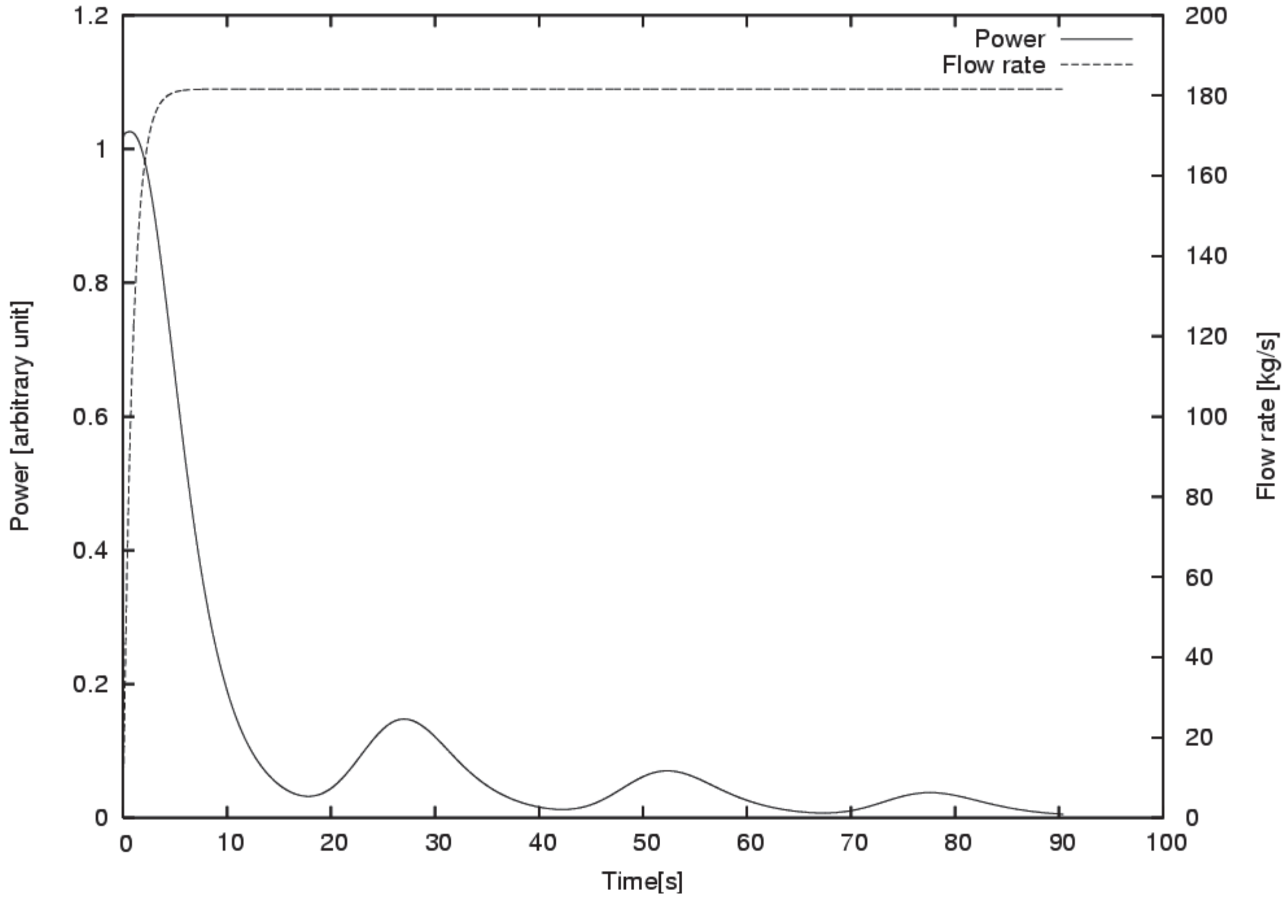
MSRE: Dynamic coupling

- Explicit scheme
- Exchange of power and temperature
- THERM and DALTON calculate each step separately
- Communicate afterwards

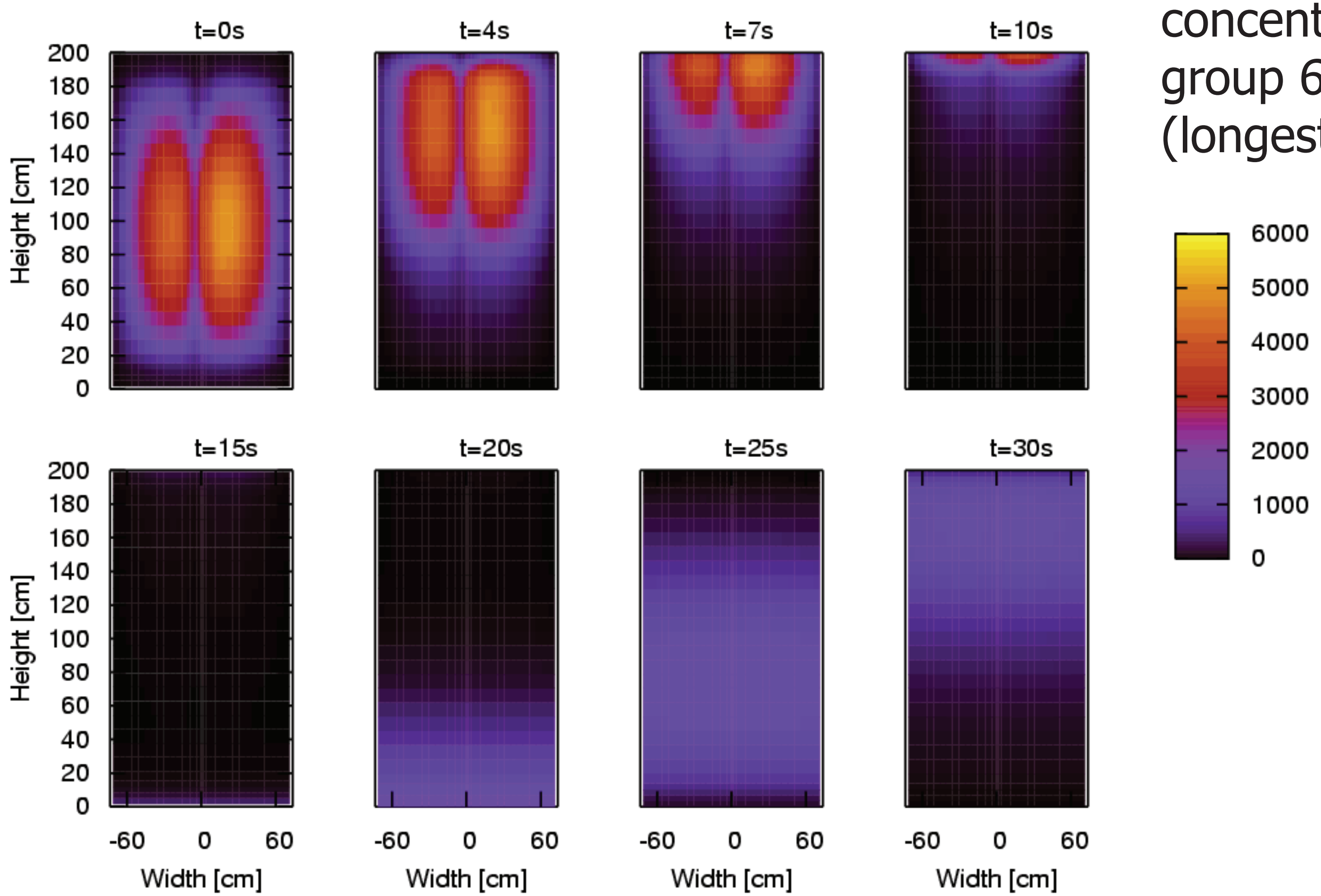


MSRE: Pump start-up

- Typical fluid-fuel transient
- Power: 1W
  no feedback
- Beginning:
  - fuel stationary
  - $k_{eff} = 1$
- Starting fuel pump



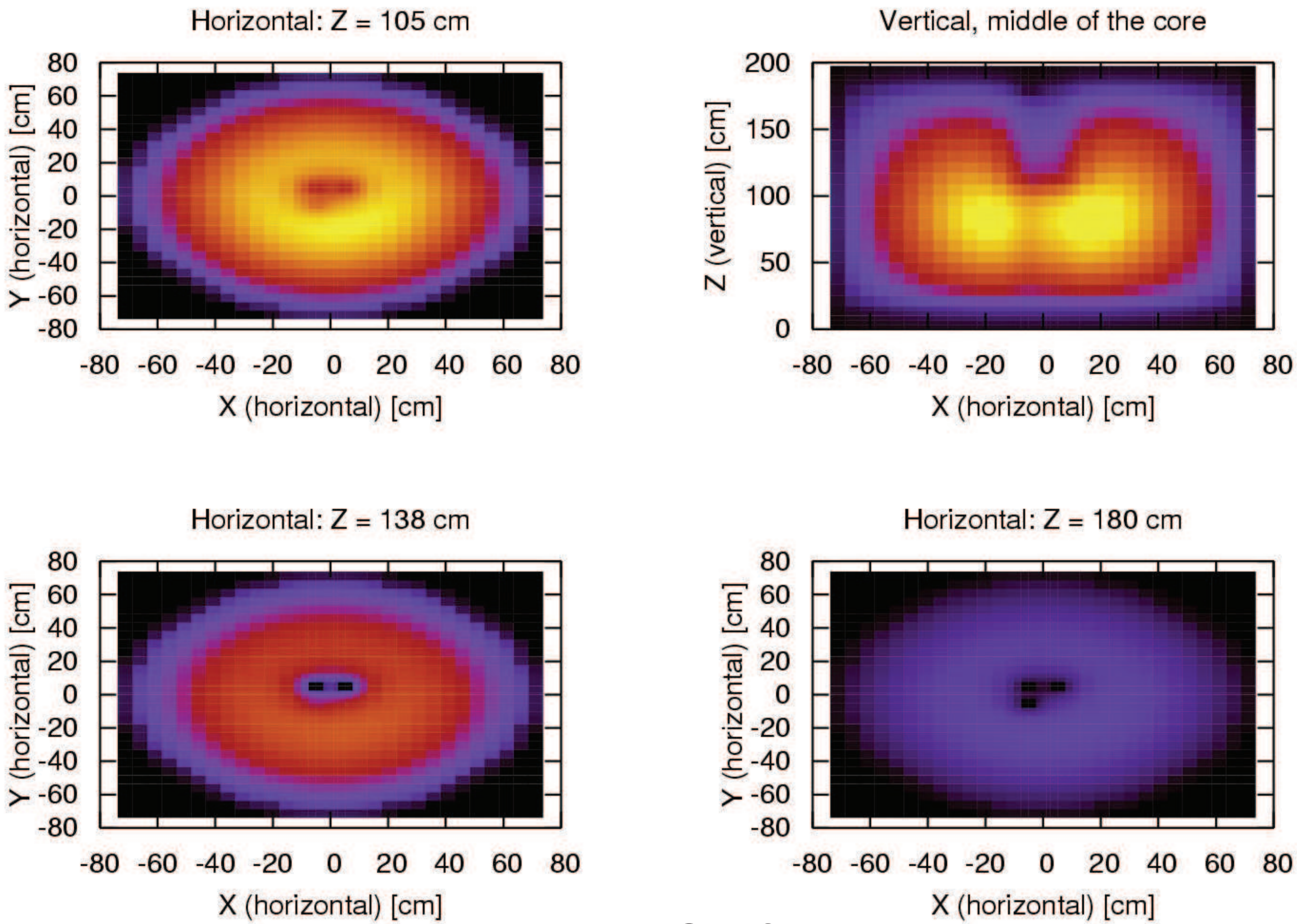
MSRE: Pump start-up



Precursor concentration group 6 (longest $T_{1/2}$)

SAMOFAR

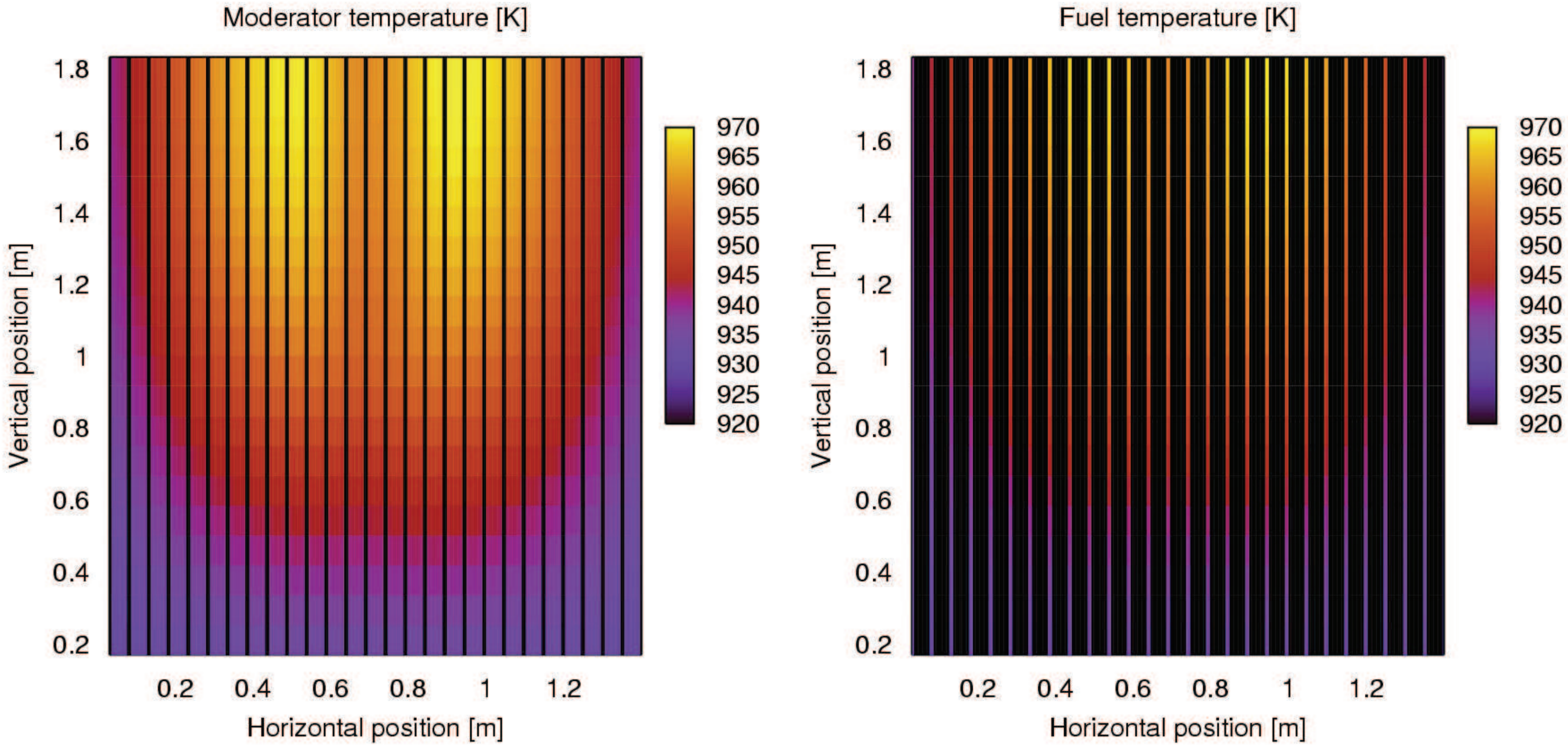
MSRE: Thermal flux (static)



power 8.59 MW

SAMOFAR

MSRE: Temperature (static)

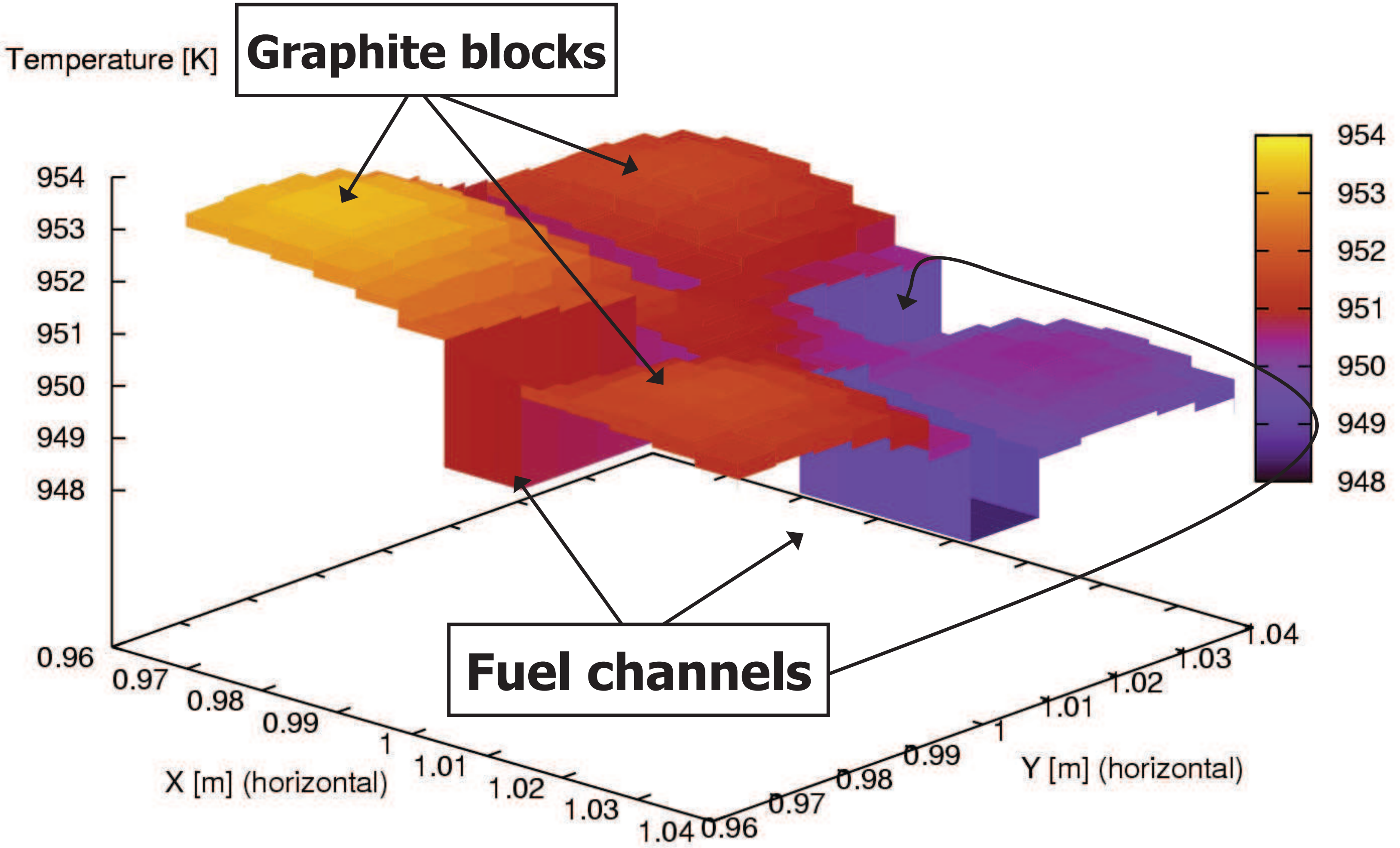


power 8.59 MW

SAMOFAR

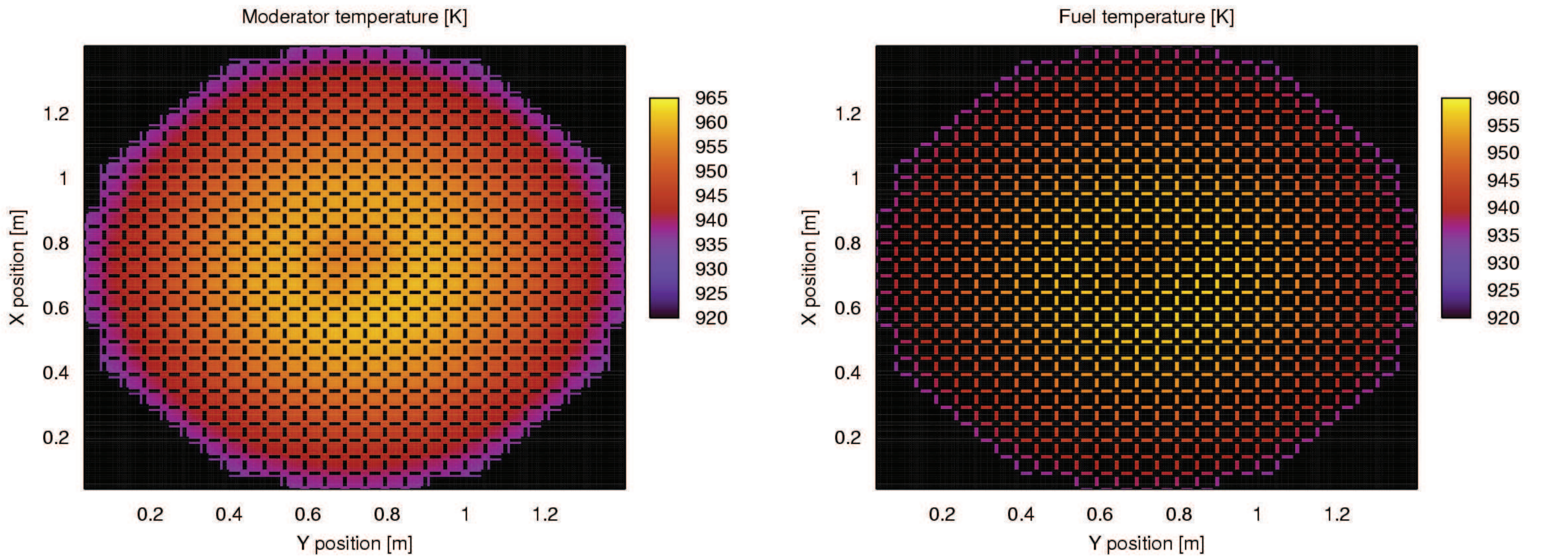
MSRE: Temperature field close-up

High resolution calculation to determine the surface temperature of the graphite and the heat transfer



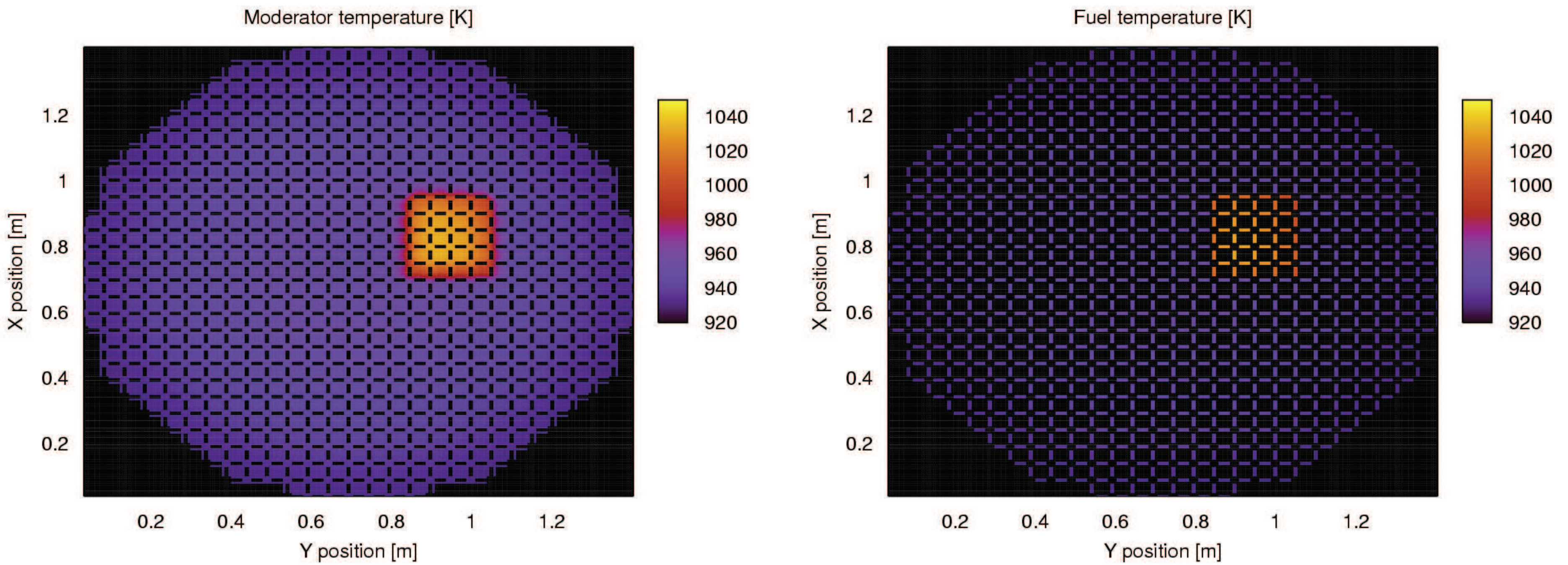
MSRE: Temperature field (static)

Horizontal cross-sectional of temperature fields at the middle of the core



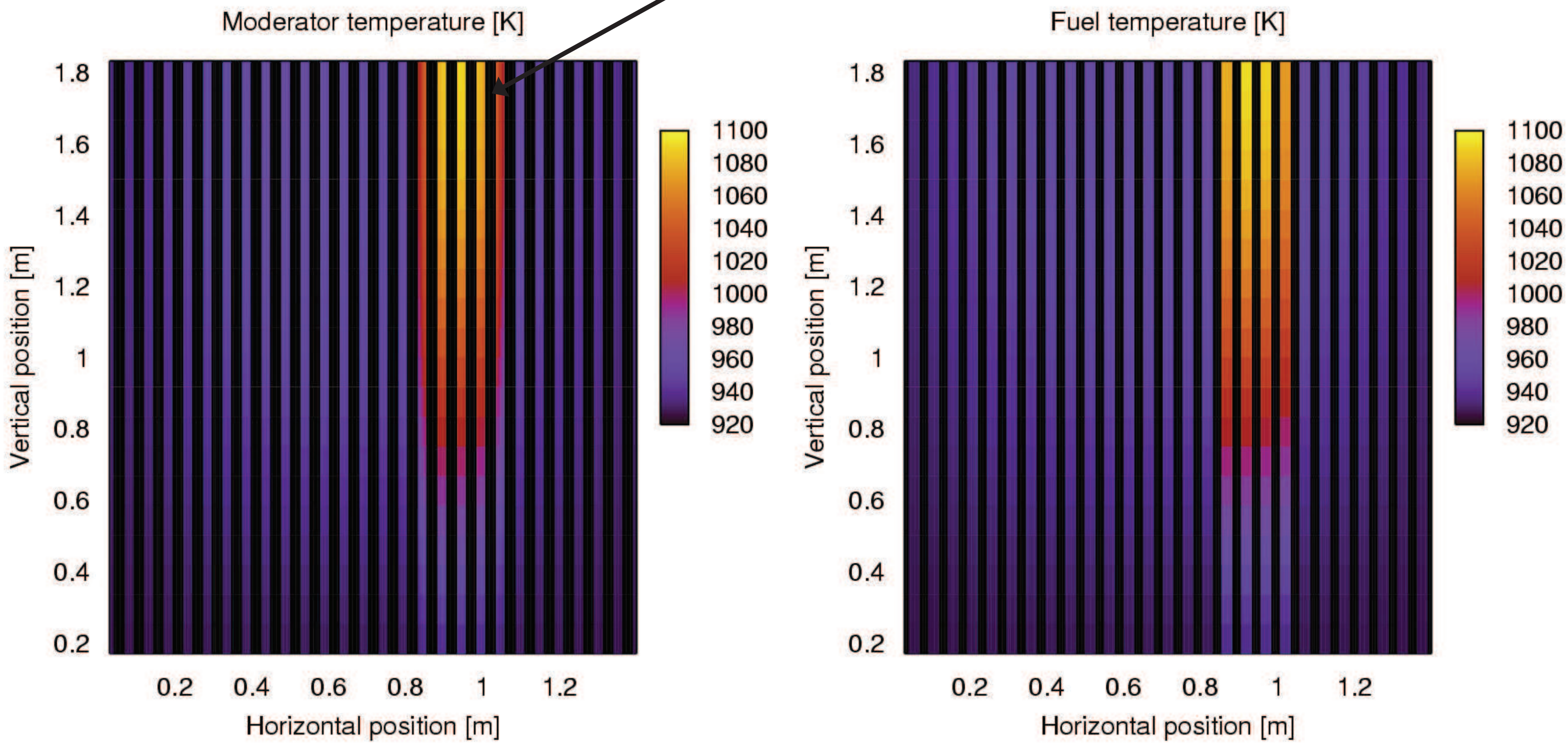
MSRE: Debris accident

- Debris gets into primary loop
- Blocks some of the fuel channels – mass flow reduced by 80%
- Total mass flow maintained
- Power reduces: 8.59 MW → 8.32 MW



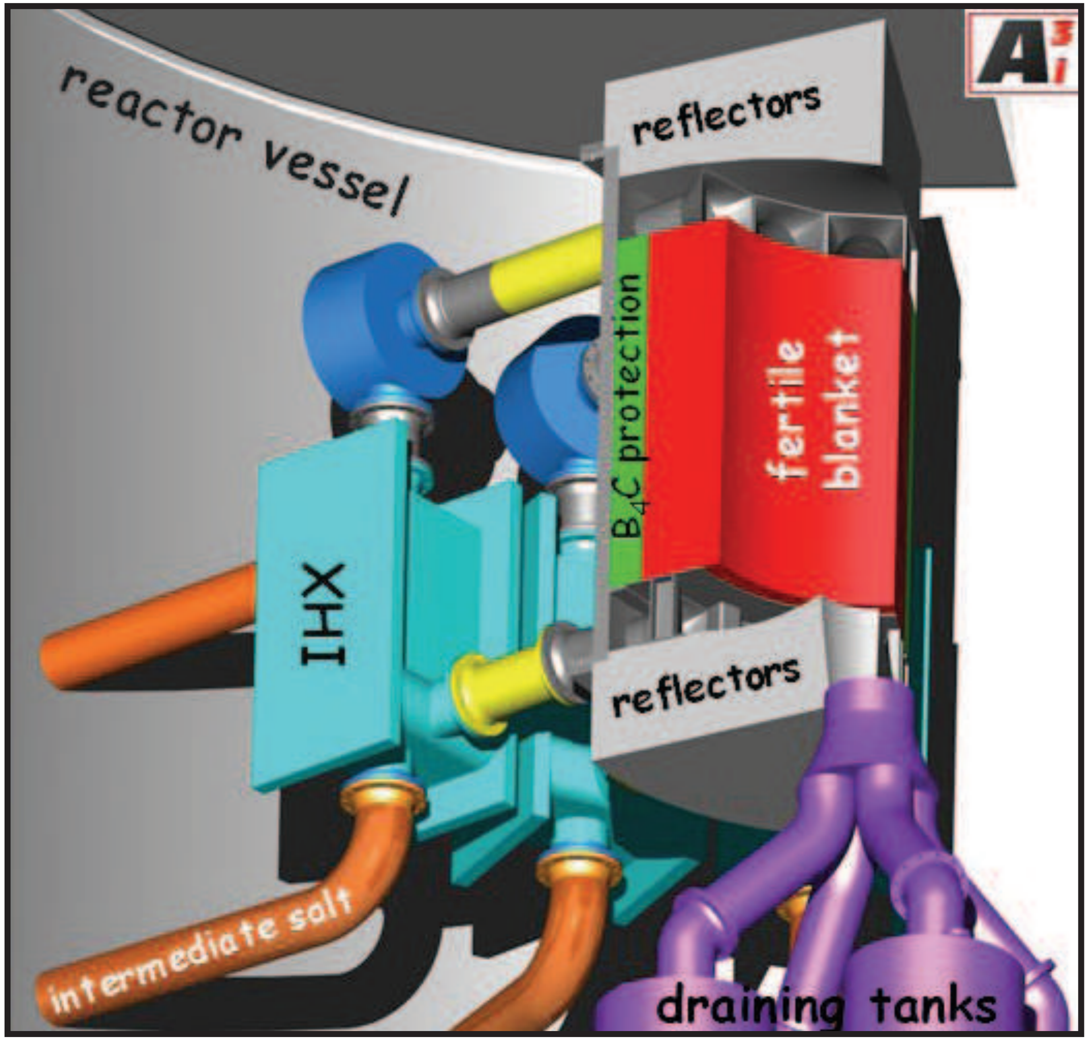
MSRE: Debris accident

Graphite conducts the heat from blocked channels



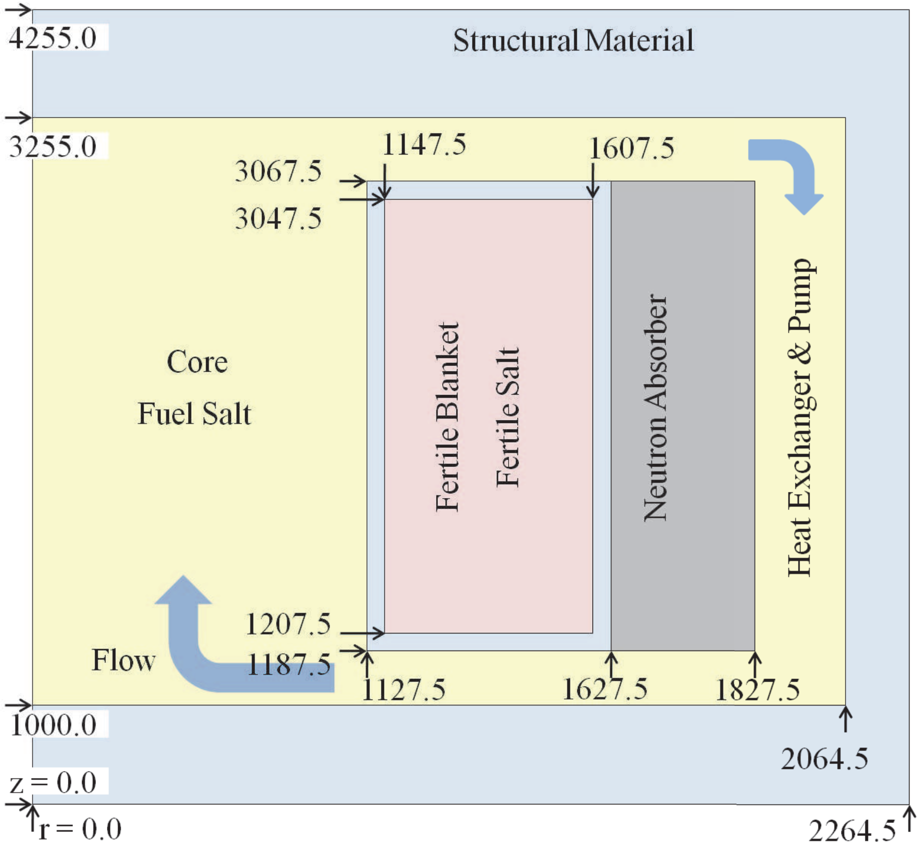
SAMOFAR

Molten Salt Fast Reactor (EVOL project)



SAMOFAR

MSFR: Geometry and physics



Modeling:

- No heat transfer in blanket, reflectors and absorber regions
- Fresh fuel
- No flow in blanket
- Complete rz models for neutronics and heat transfer and fluid dynamics
- Properties from benchmark description (except 'Boussinesq' and some simplified materials)

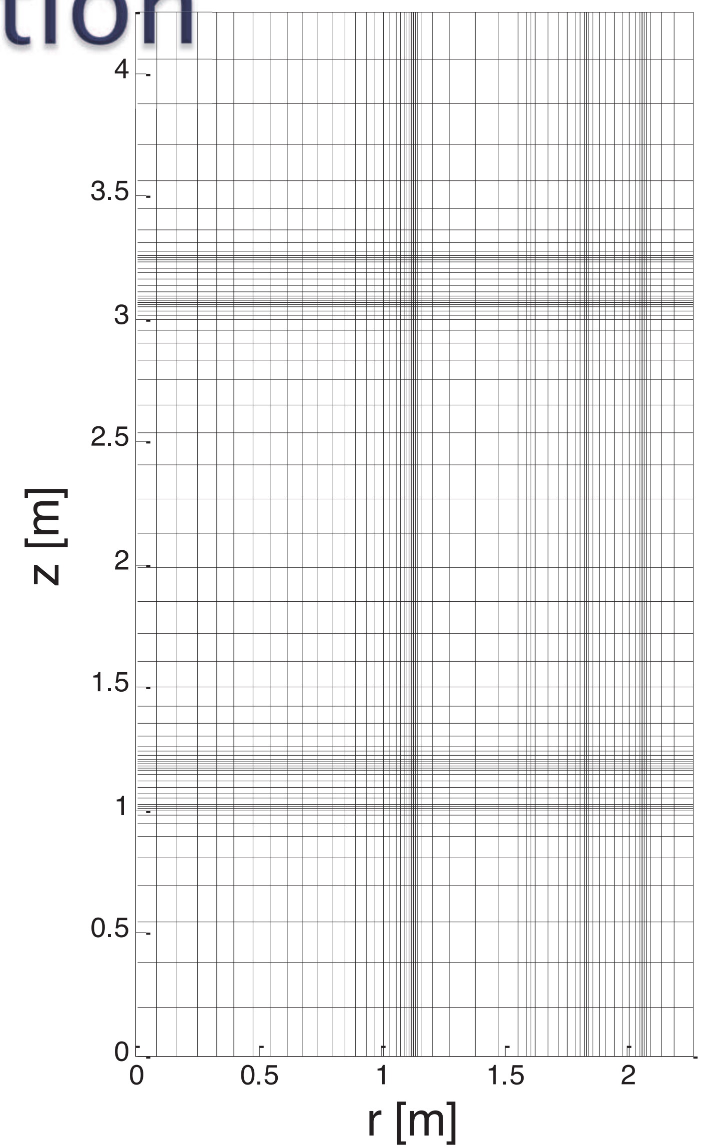
MSFR: Mesh generation

Computational mesh for neutronics 66x78

CFD mesh twice as fine in each direction (132x156). Has proper width near walls for correct behavior of turbulence model, i.e. y^+ values (friction, turbulence)

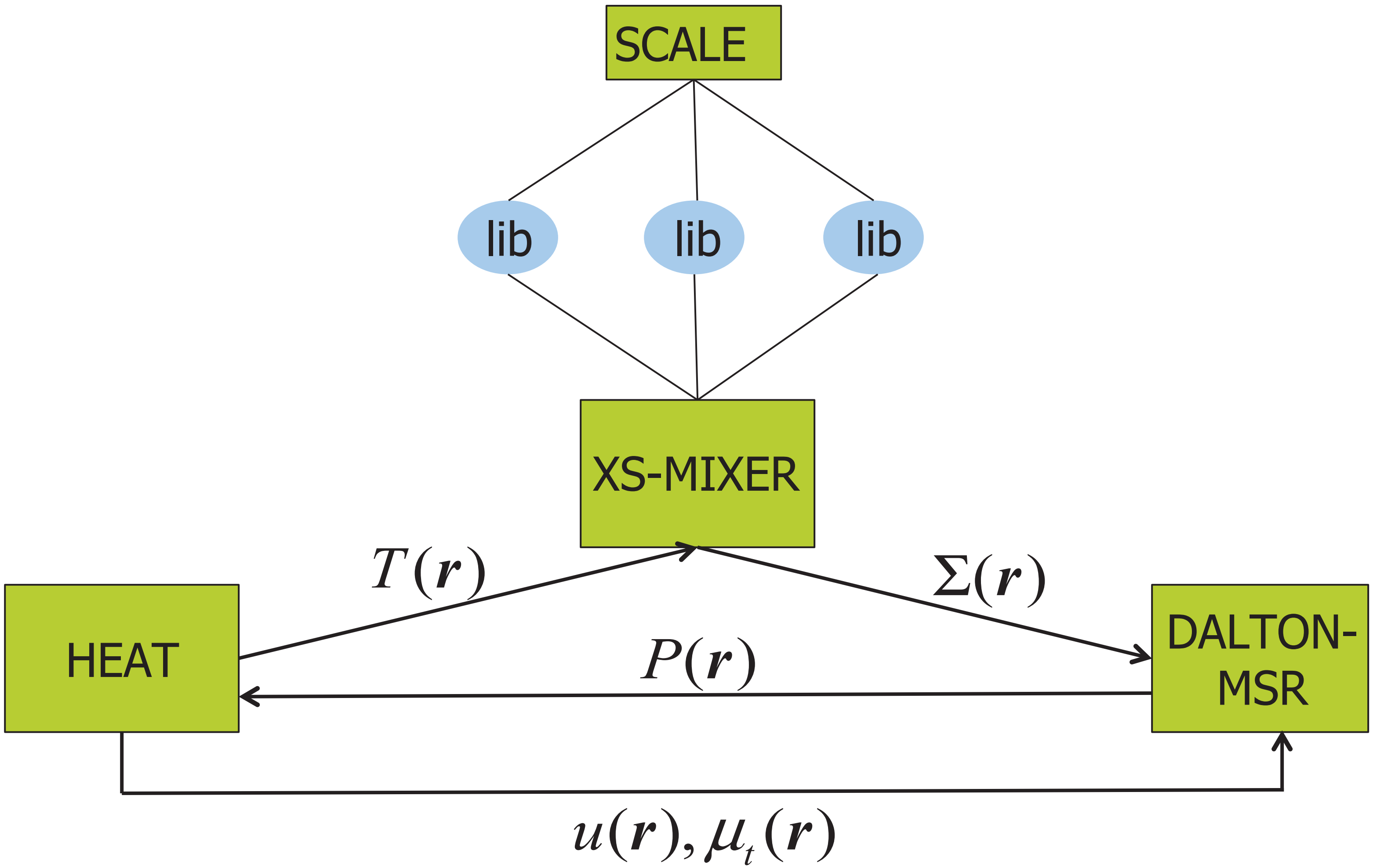
Meshes overlap for simplicity where CFD dictates refinement near walls

Interpolations required for data transfer between codes (conservation issue)

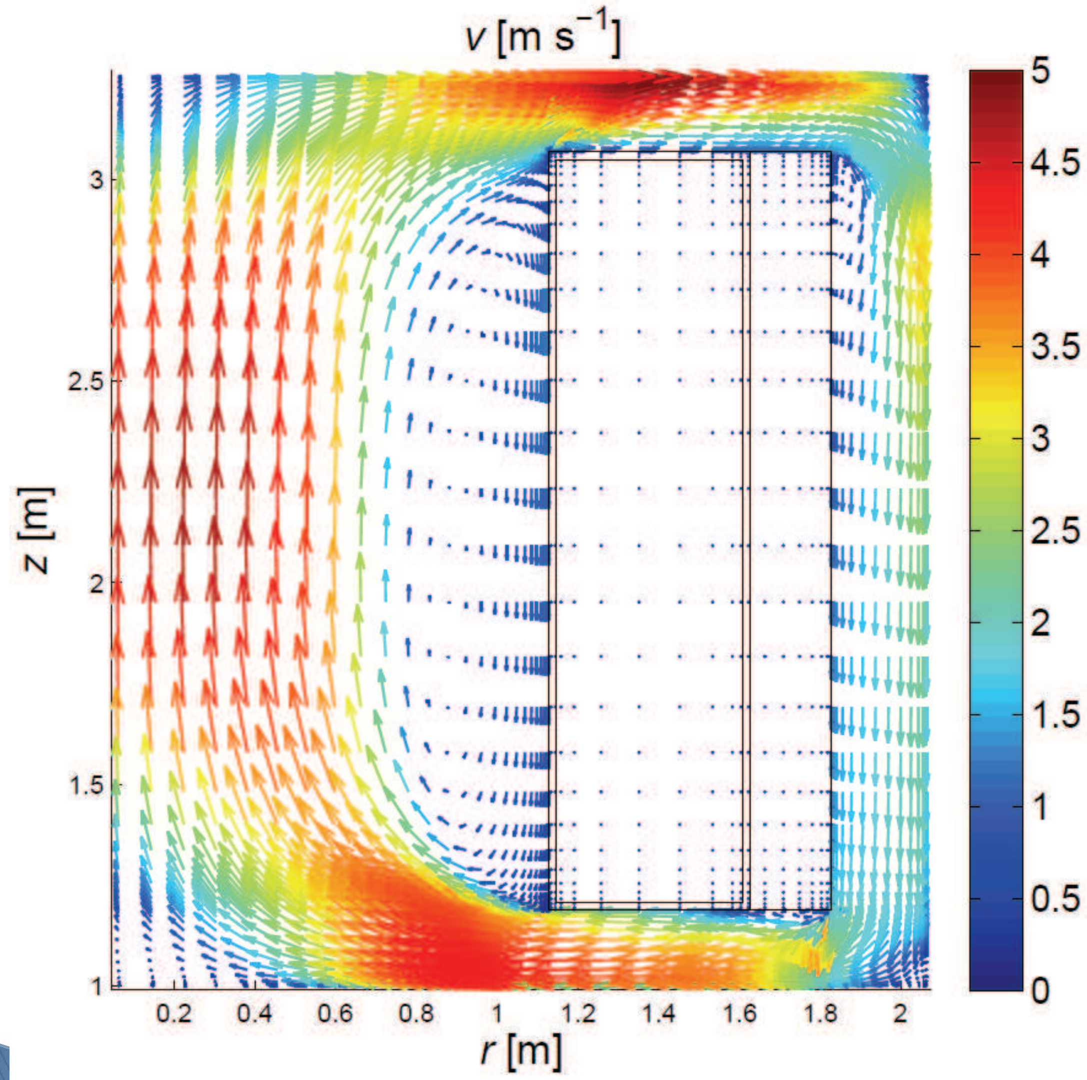


SAMOFAR

MSFR: Computational scheme

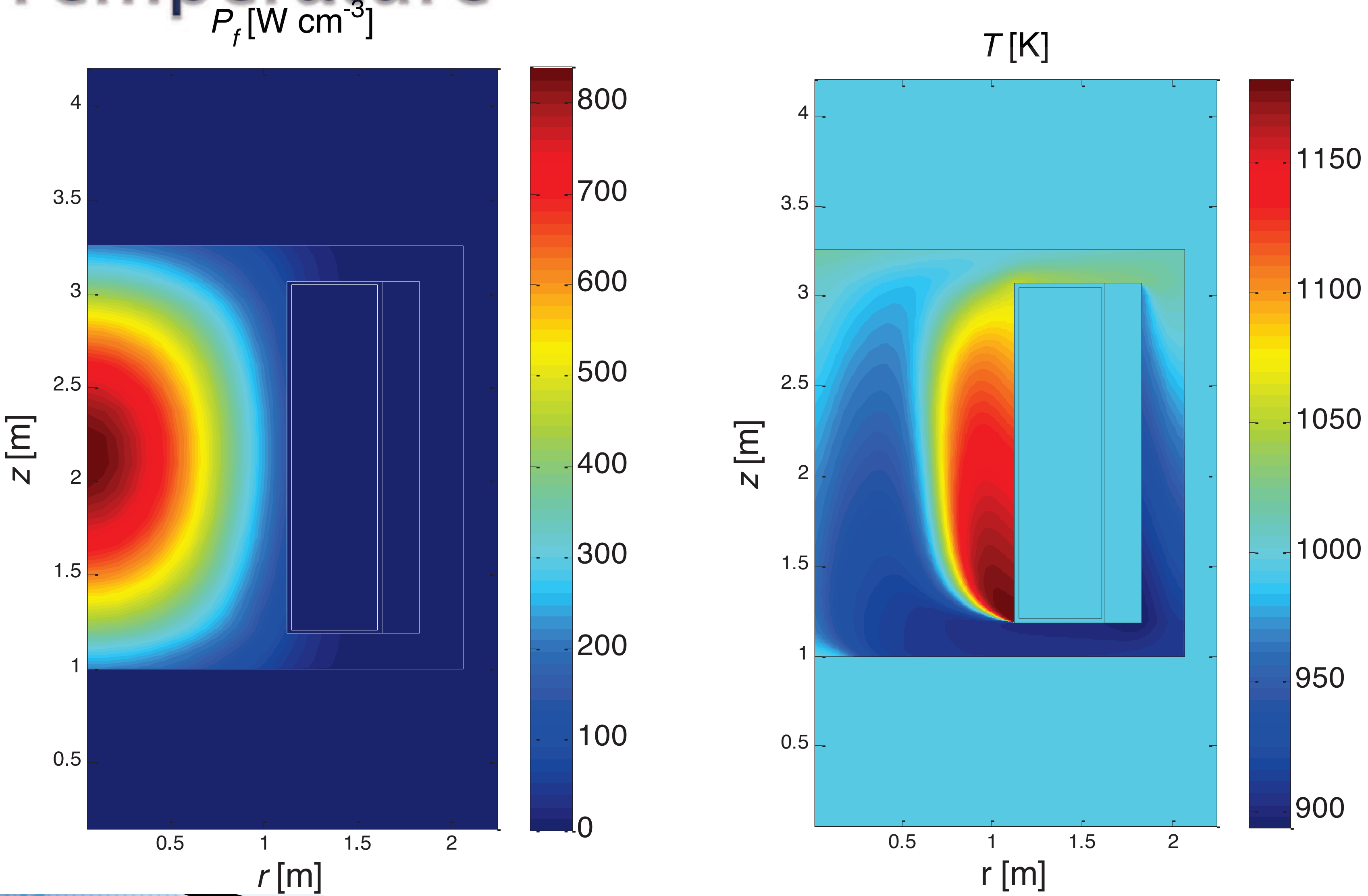


MSFR: Steady state, mean flow



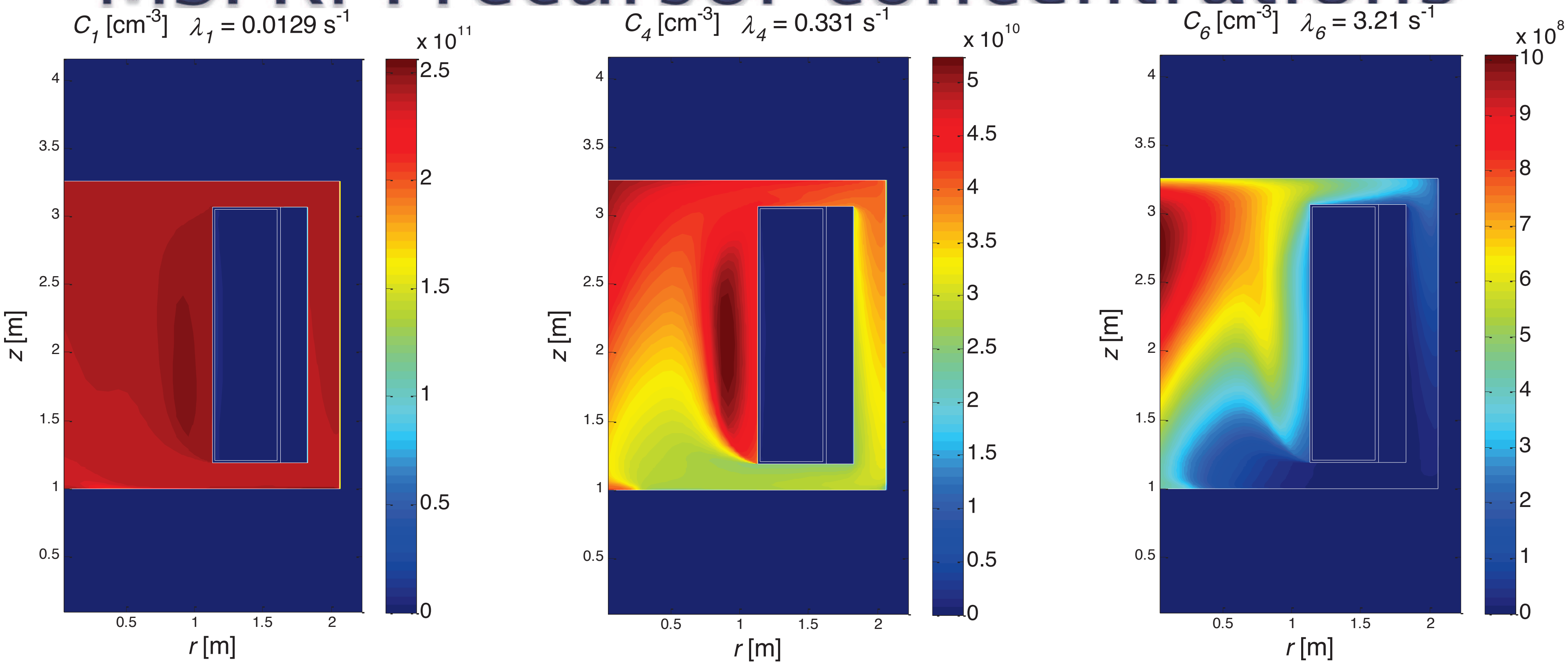
- Main recirculation loop: disadvantage for temperature field
- Small secondary flow in corner regions

MSFR: Steady state, Power density, Temperature



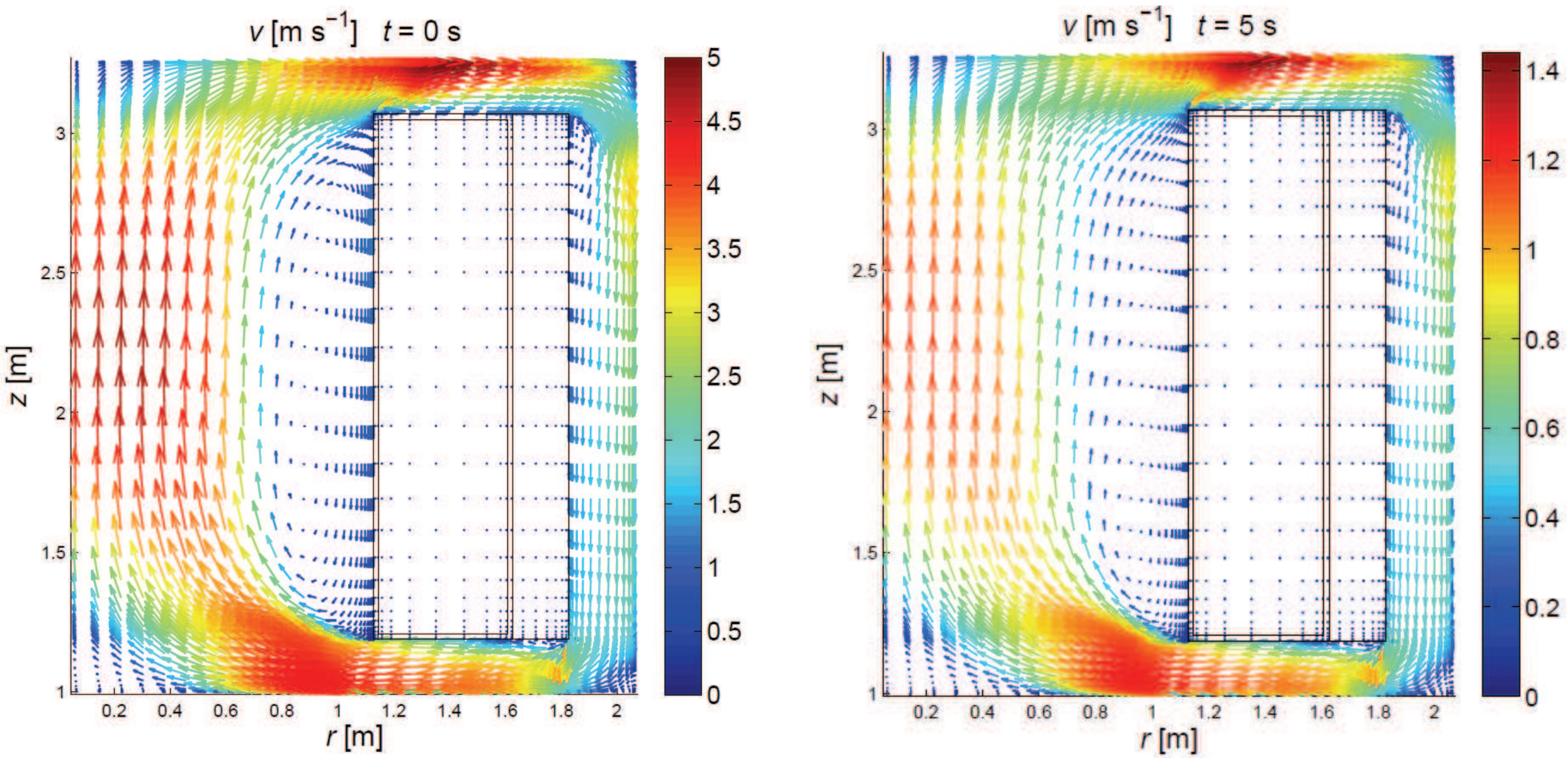
SAMOFAR

MSFR: Precursor concentrations



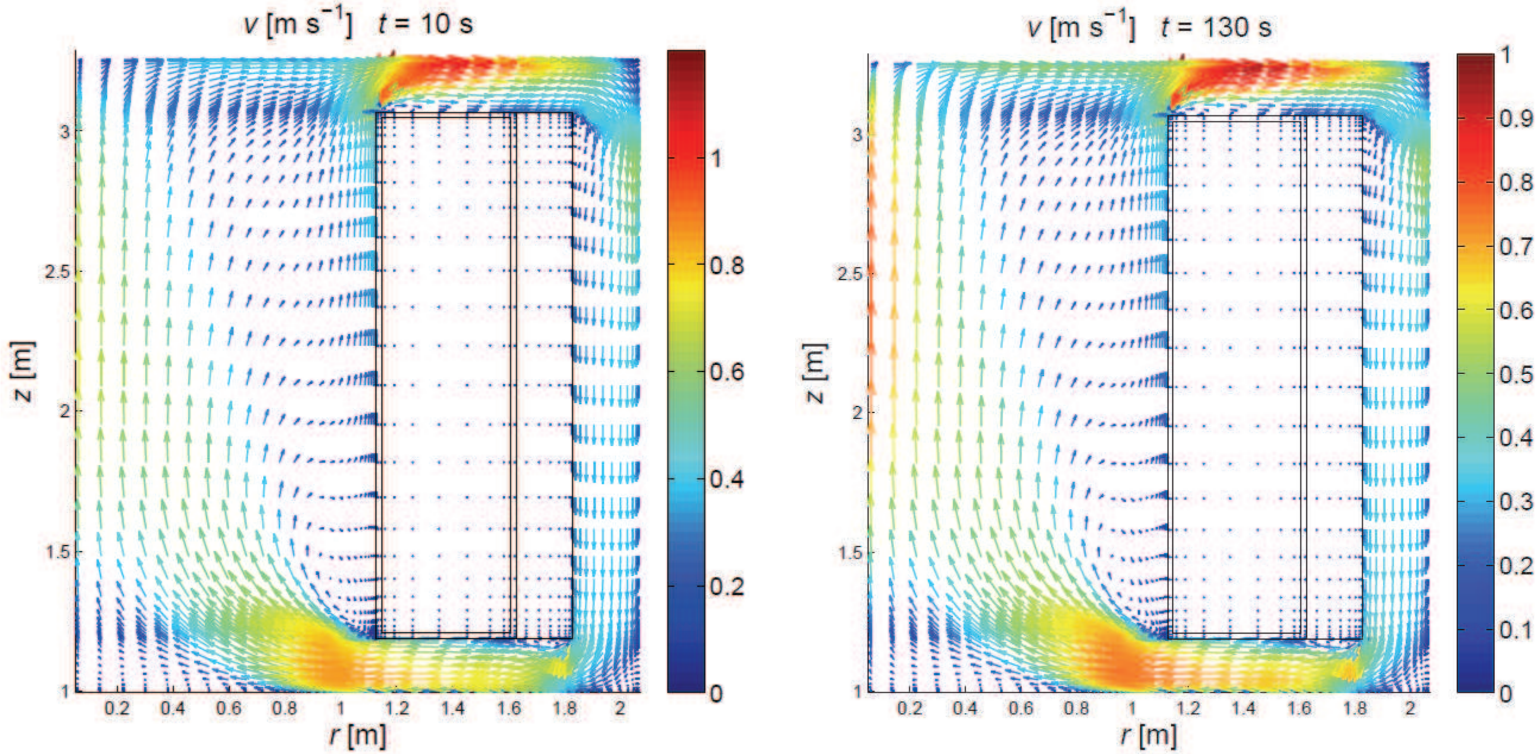
- Long lifetimes: homogeneous distributions and decay.
- Short lifetimes: local balance between production and decay. Only slight shift in spatial distribution. Complete decay in down comer.
- Intermediate lifetimes: mixed …

MSFR: Pump failure



- Rapid initial decay of flow rate within first 5 seconds

MSFR: Pump failure



- Flow almost steady state after 130 seconds
- Flow rate decreased by factor 6 compared to steady-state
- Pure natural convection with different structure of recirculation zone
- Complex interplay between flow and buoyancy

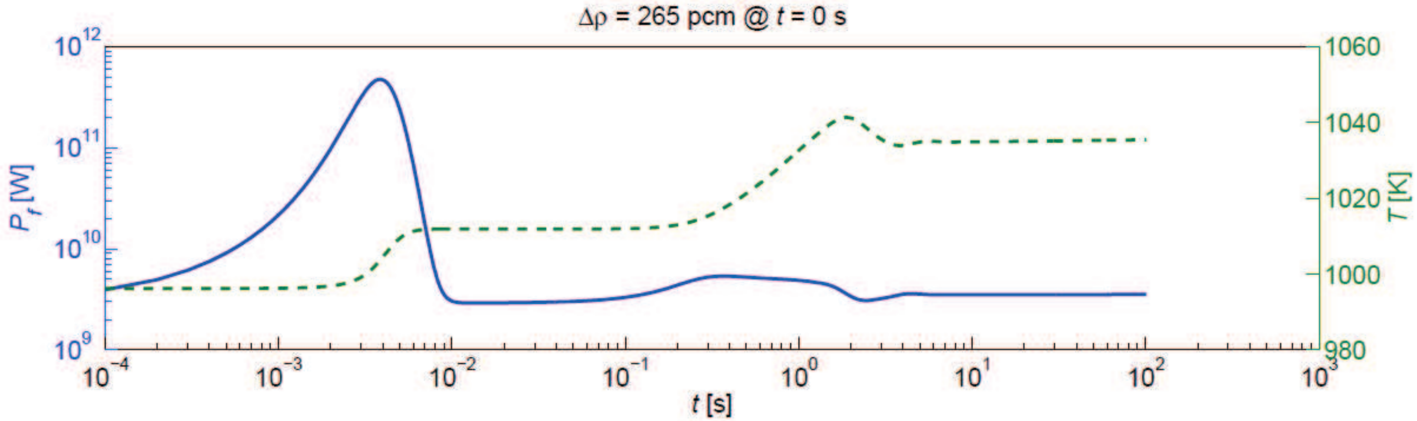
SAMOFAR

MSFR: Reactivity insertion

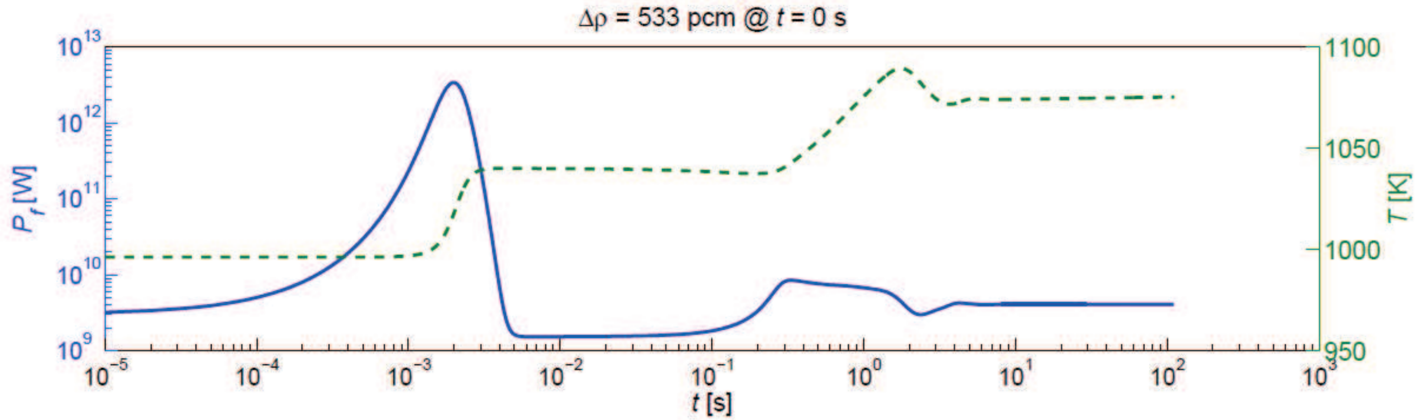
Sequence of events

- Reactivity is instantaneously added by increasing U-233 density
- ‘Prompt jump’ occurs, where feedback limits the growth
- Delayed effects from precursors
- Complex interplay of hot and cold fluid exiting and entering the core region cause some further transients until final steady state is reached
- The final power in steady state is slightly larger than the initial power to compensate for the external reactivity

MSFR: Reactivity insertion



(d) For the new steady state $P_f = 3.5$ GW and $T = 1035$ K.



(e) For the new steady state $P_f = 4.1$ GW and $T = 1075$ K.

SAMOFAR

Conclusions on multi-physics modeling

- High-fidelity code systems are available for MSR systems (Delft, Milan, PSI, CNRS, KIT, etc)
- Realism of the simulations is continuously increasing (geometric complexity, physics)
- Indispensible tool for safety analysis of MSR
- Still immense computational problem
- Future holds more
  - Chemistry coupling
  - Structural analysis
  - …

SAMOFAR

Some of our publications on MSR

- J. Kophazi et al. Development of a three-dimensional time-dependent calculation scheme for molten salt reactors and validation of the measurement data of the molten salt reactor experiment Nucl. Sci. Eng 163(2), pp 118-131, 2009.

- C. Fiorina et al. Modeling and analysis of the MSFR transient behaviour. Annals of Nucl. Energy 264 (485-498), 2014.

- K. Nagy. Dynamics and fuel cycle analysis of a moderated molten salt reactor. PhD thesis. + his papers

- Master theses Michiel Hoogmoed, Erik van der Linden, Lodewijk Frima.

- Downloads at https://www.tudelft.nl/en/faculty-of-applied-sciences/about-faculty/departments/radiation-science-technology/kloosterman-group/publications/

SAMOFAR


Q
&
A