Modelling frozen salt walls in molten salt fast reactors

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Overview

1. Molten Salt Fast Reactors
2. Modelling Frozen Walls using a porous medium approach
    - 2D Differentially Heated Cavity
3. Application to MSFRs
    - Coupled Methodology
    - Results
4. Conclusions and Future Work

Overview

Background

Molten Salt Reactors

- Developed from '40s to '70s by Oak Ridge National Laboratory
- Fuel is dissolved in salt (FLiBe) and pumped through a graphite moderated core region
- Operated at 650 °C ^{235}U/^{232}Th and it bred ^{233}U.

`http://energyfromthorium.com/msrp/http://moltensalt.org`

Molten Salt Fast Reactors

- One of six Generation-IV reactor concepts to develop efficient, sustainable and safer fission reactors
- Design concepts are based on reactors with no core internals
- Operating temperature 890 K to 1100 K
- Breed ^{233}U from ^{232}Th
- Burn plutonium

`https://www.gen-4.org/gif/jcms/c_42150/molten-salt-reactor-msr`

Background

Pros

- \+ Inherently safer
- \+ **Molten core**
- \+ Atmospheric pressure
- \+ Strongly negative reactivity coefficient
- \+ Continuous feed and recycling of fuel-salt
- \+ Remove volatile fission products and neutron poisons
- \+ Lack of minor actinides in waste could reduce storage time <1000 years
- \+ Smaller quantities of long-lived fission product waste

Cons

- **Corrosion**
  - Salt attacks nickel based alloys used in structural materials
  - Shortens safe lifespan
- High neutron flux
  - Nuclear reactions with isotopes in vessel wall
  - Nickel isotopes evolve helium
  - Helium embrittles the walls
- Pre- and post- processing techniques for the fuel and fission products are immature
- New safety concepts are required - lowest layer of defense-in-depth removed

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Equations for a liquid-solid phase change

The starting point are the Navier-Stokes-Fourier equations

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \\ \dfrac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla P + \nabla \cdot \tau + \rho \mathbf{g} + \nabla \cdot (\rho \mathbf{R}) + \mathbf{s_u} \\ \dfrac{\partial \rho c_p T}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla \cdot (k_{eff} \nabla T) - s_T \end{cases}$$

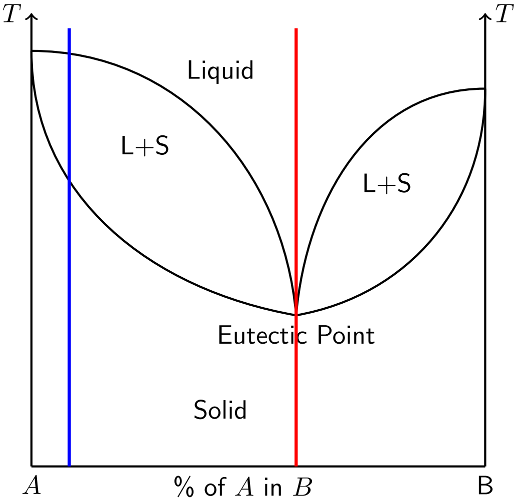
with

- $\tau = \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T - \dfrac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right)$
- $\rho \mathbf{R} = -\mu_T \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T - \dfrac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \dfrac{2}{3} \rho k \mathbf{I}$

Two extra source terms are present to take into the phase change and precisely

- $\mathbf{s_u}$ the account for the porosity of the medium
- s_T the Latent Heat of the phase change

2-component phase diagram



- Our salt can be considered a 2-component material with a fix concentration of A into B
- The phase can be generally defined by the liquid fraction χ defined as

$$\chi = \begin{cases} 0 & \text{For solid} \\ \dfrac{T - T_S}{T_L - T_s} & \text{For L+S} \\ 1 & \text{For liquid} \end{cases}$$

- Linear variation of χ with T is assumed for simplicity
- At Eutectic point $T_L = T_S$ and χ assume only values 0 (solid) or 1 (liquid)

Phase-change terms

Porous medium approach

$$\mathbf{s_u} = -A\mathbf{u} = -\frac{-C\left(1-\chi\right)^2}{\chi^3+q}\mathbf{u}$$

- Formulation of the term is derived from Darcy's law
- C and q depends on the morphology of the porous medium:

Latent heat

$$s_T = \underbrace{\frac{\partial\left(\rho\chi L\right)}{\partial t}}_{\text{Transient}} + \underbrace{\nabla\cdot\left(\rho\chi L\mathbf{u}\right)}_{\text{Convective}}$$

- The term is composed by a time dependant and a convective terms
- Convective term is discretised using a fully first order up-wind scheme
- The transient term is recast in term of T and therefore can be partially implicited at T^{n+1}

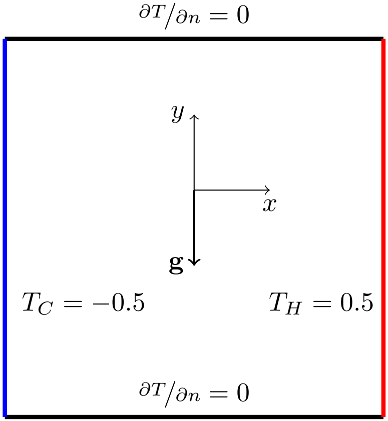
Test-case definition

2D laminar test[1]case with constant fluid properties

- $Ra = 10^4$, $Pr = 10^3$
- Stefan number Ste

$$Ste = \frac{c_p(T_H - T_C)}{L} = 5$$

  with L being the latent heat
- $T_L = -T_S = 0.1,\ 0.05, 0.0$ (last not yet tested)
- Boussinesq approximation for the buoyancy term
- Structured and uniform grid 64×64



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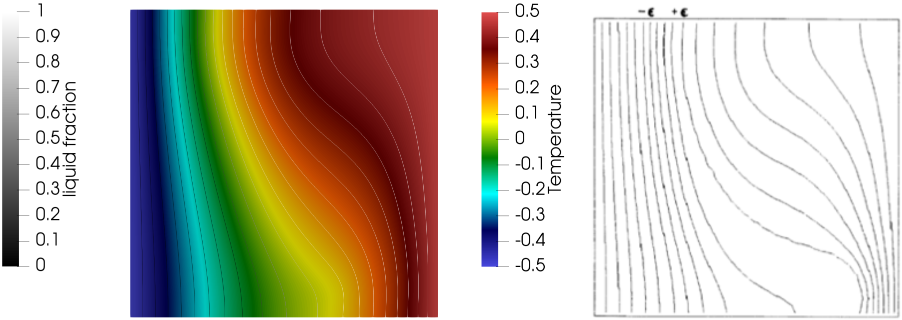
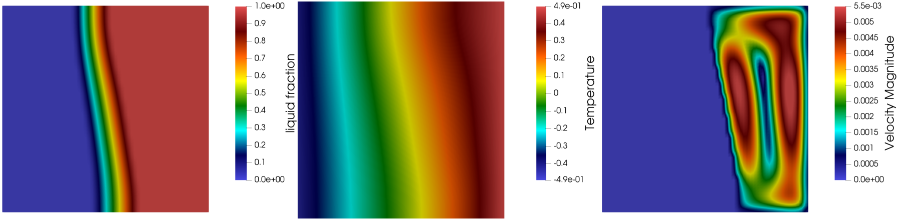
[1] A fixed grid numerical modelling methodology for convection-diffusion mushy region phase-change problems, International Journal of Heat and Mass Transfer

Results: Comparison with *Voller & Prakash*

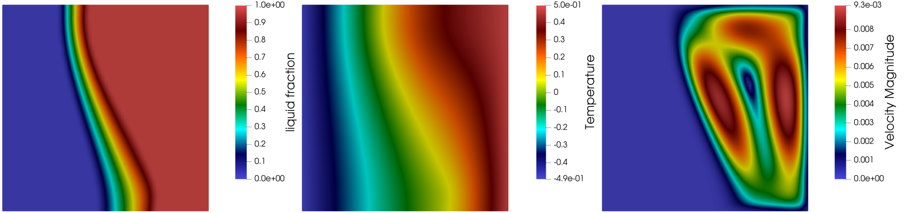


Results:
Variation of C and q

$C = 10^{10}$ and $q = 10^{-6}$



$C = 1.6 \cdot 10^3$ and $q = 10^{-3}$ (Reference values from *Voller and Prakash*, 1987)



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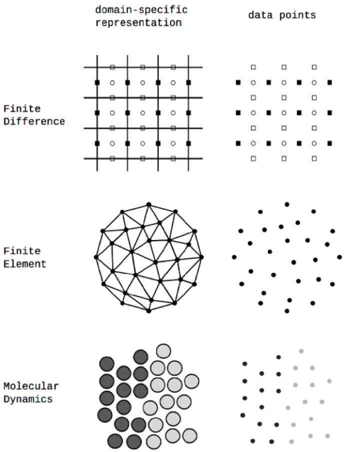
MSFR: Test case definition

- Reactor design characterised by 16 primary circuits
- 2D and 3D geometries with and without heat exchanger have been tested
    - Block structured
    - 2D meshes size from 95,000 to 330,000 cells
    - 3D meshes starting from 5M cells
    - First cells at the wall is 0.001 mm which gives a max $T^+ \approx 0.3$
    - At least 35 nodes are used in the first 40 mm
- Full variation of fluid properties as function of the temperature
- BL-v^2/k RANS turbulence model used
- Analytical definition of the heat source in the core of the reactor
- For the geometry without the heat exchanger a fully developed profile with a bulk temperature $T_B = 898\,\mathrm{K}$
- Lithium fluoride salt with thorium (Li_3ThF_7)
- **Conjugate Heat transfer using internal *Code_Saturne* coupling (2D)**
- **Coupled neutronics calculations with DYN3D-MG using Multiscale Universal Interface (MUI) for the code couplig(only 3D)**

MUI[2]: Multiscale Universal Interface

- Header-only C++ library, couples using a set of discrete data samples and **interface**
  1. Convert domain-specific representations (i.e. mesh) to general form (i.e. a cloud of data points)
  2. Solver imparts data (at a point in space) to MUI interface with an associated time-stamp
  3. Other solver requests data at specific location and time from MUI interface using spatial and temporal sampler
  4. It is possible to make it conservative (radial basis function interpolation)
- Uses MPI MPMD
- Developed initially to couple multi-scale (particle based) methods



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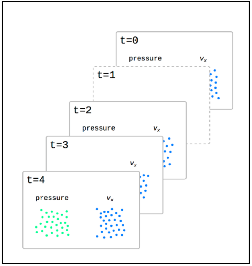
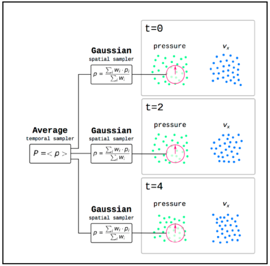
[2] Multiscale Universal Interface: a concurrent framework for coupling heterogeneous solvers YH Tang, S Kudo, X Bian, Z Li, GE Karniadakis - Journal of Computational Physics, 2015

MUI: Multiscale Universal Interface

SOLVER A



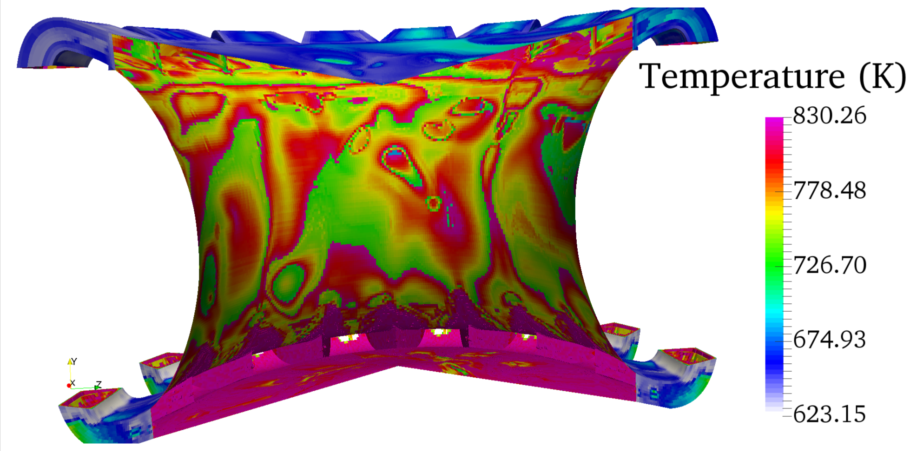
SOLVER B



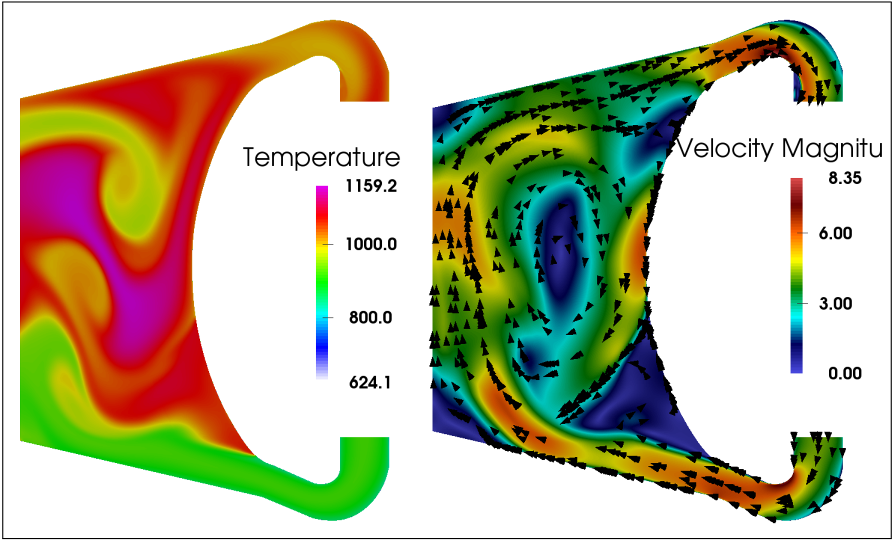
```
#include "mui.h"
uniface interface("mpi
␣␣␣␣␣␣␣␣␣://domainA/interface1" );
for( t=0; t<T; t+=dt_A ) {
  [compute u, v, w, p, etc.];
  for(all points in send region){
    interface.push( "label",
    point, data);
  }
  interface.commit( time=t );
}
```

```
#include "mui.h"
spatialSampler ss();
temporalSampler ts();
uniface interface("mpi
␣␣␣␣␣␣␣␣␣://domainB/interface1");
for( t=0; t<T; t+=dt_B ) {
  for(all points on coupled boundary){
    data = interface.fetch( "label",
           point ,time, ss, ts );
  }
  [compute u, v, w, p, etc.];
}
```

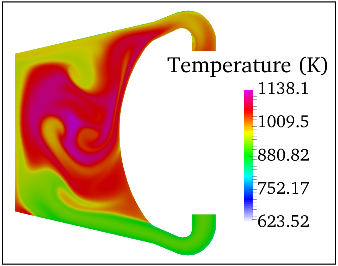
MSFR:
3D Full geometry

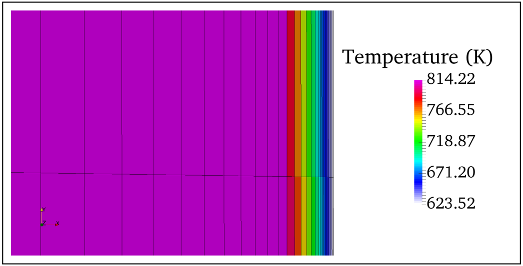


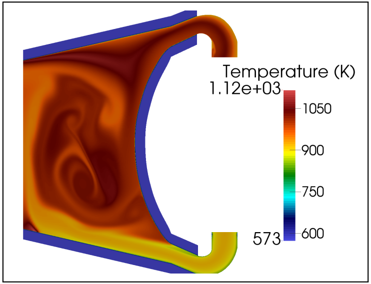
MSFR:
Basic 2D geometry

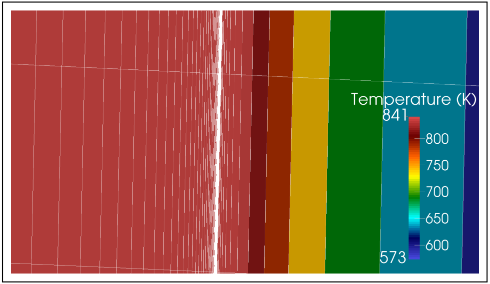


MSFR 2D: with and without conjugate heat transfer









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In Summary

- A multi-physics framework that uses conjugate heat transfer, a porosity base model for liquid-solid phase changes together coupled with a neutronic transport model has been developed to simulate molten salt fast reactors
- The model has been used to investigate the formation of a frozen salt film to protect the vessel from corrosion, finding the formation of the film is greatly impaired by the very small thermal boundary layer
- A framework for code-coupling for multi-scale-physics simulations is in development and based on the MUI library

Current Work

- Further calculations are necessary on a large 3D geometry to further validate the finding
- More work towards validation is necessary mainly in the area of very turbulent flows with solid-liquid phase transition

Acknowledgements

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