

SERPENT workshop
Berkeley,
6-8 November 2013

Recent Serpent-related works at Politecnico di Milano

Manuele Aufiero

Supervisors: prof. Antonio Cammi & prof. Lelio Luzzi



NUCLEAR REACTORS GROUP

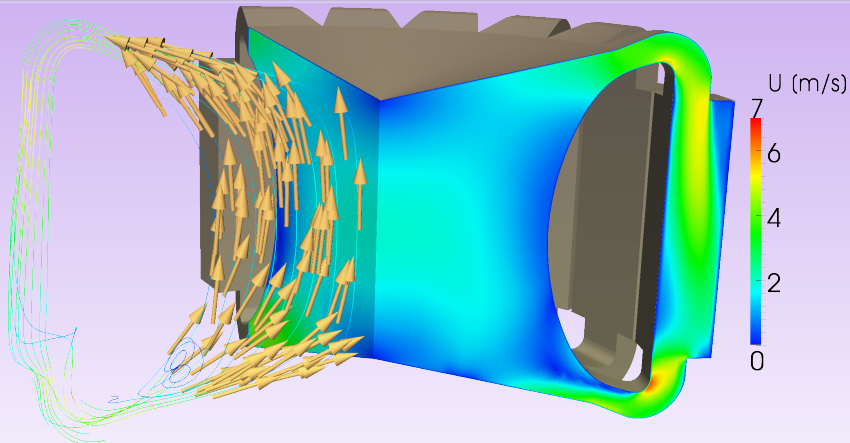
What I will talk about:

- Short background on MSR modelling
- β_{eff} calculation in circulating fuel reactors
In collaboration with LPSC – CNRS Grenoble (France) and INOPRO.
- Investigation of a possible Serpent-OpenFOAM coupling for multiphysics applications
In collaboration with FAST group @PSI (Switzerland).
- Calculation of adjoint-weighted sensitivity coefficients
In collaboration with Mathieu Hursin and Sandro Pelloni @PSI (Switzerland).



Multiphysics modelling for Molten Salt Reactors...

...coupling CFD and neutron diffusion in OpenFOAM



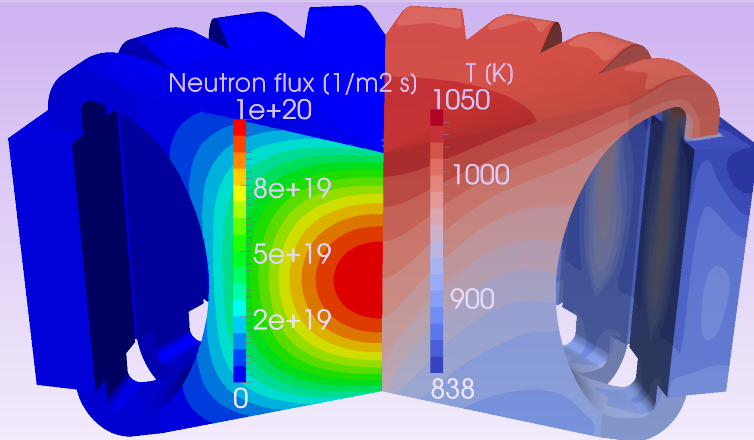
Coupled CFD/neutronics calculation for the MSFR*: velocity field

* Molten Salt Fast Reactor – EVOL Project – Euratom FP7.



Multiphysics modelling for Molten Salt Reactors...

...coupling CFD and neutron diffusion in OpenFOAM



Coupled CFD/neutronics calculation for the MSFR*: ϕ & T

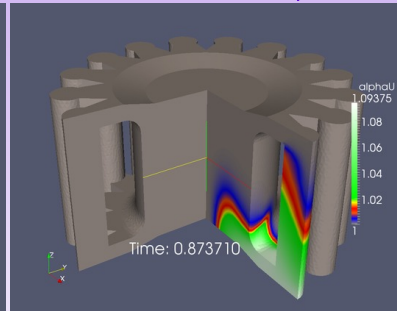
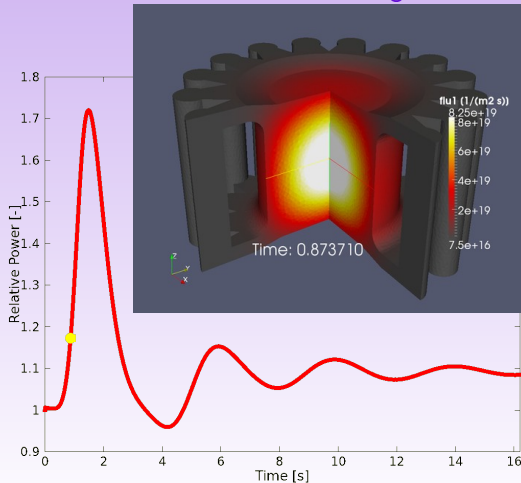
* Molten Salt Fast Reactor – EVOL Project – Euratom FP7.



Multiphysics modelling for Molten Salt Reactors...

...coupling CFD and neutron diffusion in OpenFOAM

Accidental release of ~ 15 kg of ^{233}U in one of the external loops



Multiphysics modelling for Molten Salt Reactors...

...what we still lack?

Multi-group diffusion is OK in most cases

A new discrete ordinate solver has been recently developed...

- Monte Carlo benchmark for important parameters is still highly desirable (e.g., β_{eff})
- Monte Carlo-based multiphysics modelling seems to be the best option for particular cases (e.g., small or heterogeneous MSR)



...with on-line fuel reprocessing & reactivity control

*Lanthanide series

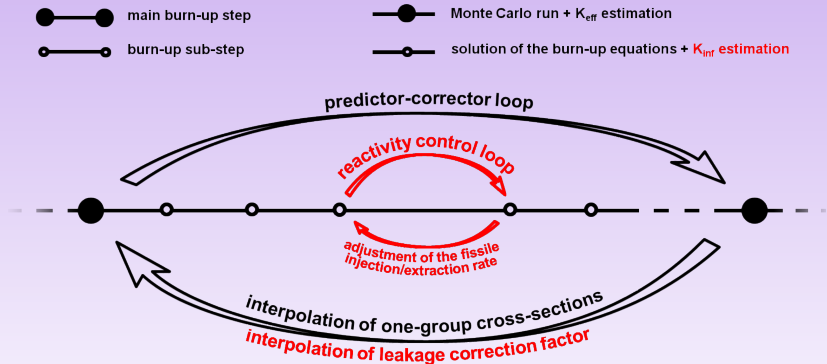
* * Actinide series

- Gaseous and not-soluble (metallic) fission products are removed by gas bubbling
- Other fission products are continuously removed by chemically reprocessing small amount of fuel salt
- The reactivity of the system is controlled by insertion/removal of Uranium
- Incineration of TRU is often considered

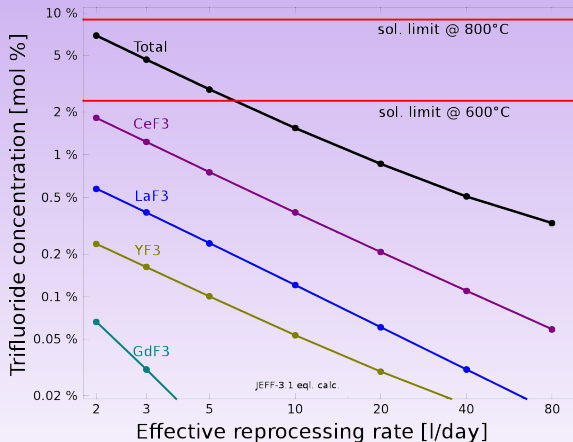


Fuel isotopic evolution & eq. calculations

...with on-line fuel reprocessing & reactivity control



Concentration of trifluorides in the MSFR @eq ...as function of the salt “clean up” reprocessing rate

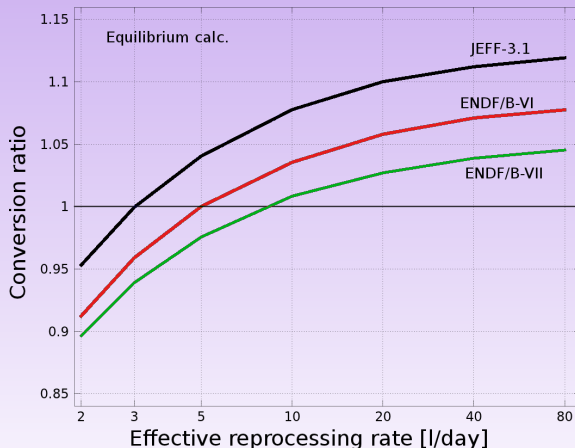


Solubility limits from:

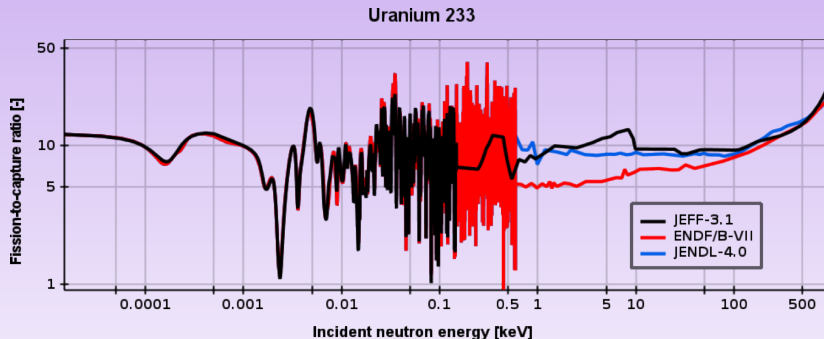
Solubility of Cerium trifluoride in molten mixture of LiF, BeF₂, and ThF₄. [ORNL-TM-2335, 1969.](#)



Conversion ratio in the MSFR @eqI for different nuclear data libraries



U^{233} capture cross-sections, where is the truth?



Fuel isotopic evolution & eql. calculations

...what we still lack?

- Impact of (large) xs uncertainties in the Th-U²³³ fuel cycle
- Impact of (large) uncertainties in on-line reprocessing removal efficiencies

first step:

- Consistent calculation of sensitivity coefficients



β_{eff} in circulating fuel conditions *

* In collaboration with LPSC – CNRS Grenoble (France) and INOPRO.

Why β_{eff} is different from β_{zero} ?

Prompt and delayed neutrons have different importance:



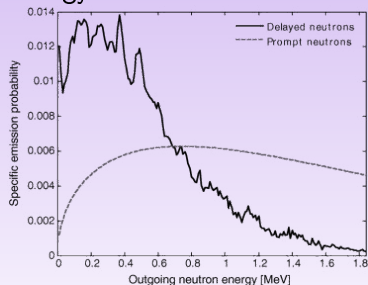
β_{eff} in circulating fuel conditions *

* In collaboration with LPSC – CNRS Grenoble (France) and INOPRO.

Why β_{eff} is different from β_{zero} ?

Prompt and delayed neutrons have different importance:

Energy effects



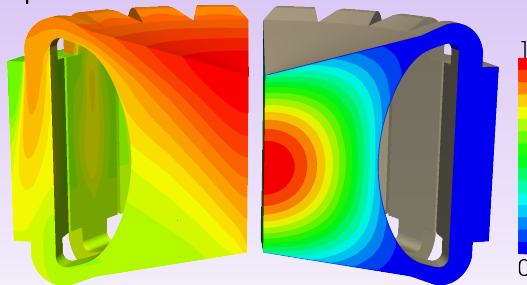
β_{eff} in circulating fuel conditions *

* In collaboration with LPSC – CNRS Grenoble (France) and INOPRO.

Why β_{eff} is different from β_{zero} ?

Prompt and delayed neutrons have different importance:

Spatial effects



Spatial distribution of the delayed (left) and prompt (right) neutron sources at nominal flow rate (arbitrary unit). OpenFOAM - 3D optimized MSFR geometry at nominal flow rate.



β_{eff} in circulating fuel conditions *

* In collaboration with LPSC – CNRS Grenoble (France) and INOPRO.

Why β_{eff} is different from β_{zero} ?

Prompt and delayed neutrons have different importance:

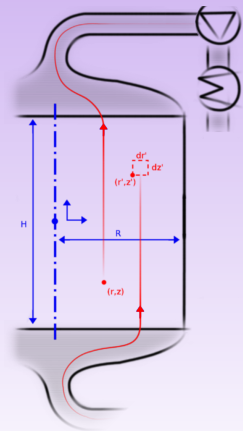
Often, β_{eff} in circulating-fuel conditions is calculated by correcting static β_{eff} , with the fraction of precursors decaying inside the core.

This might give inaccurate results due to inhomogeneous spatial neutron importance inside the core.



Simulation tools – Analytical approach

Integrating the delayed neutron source weighted with a simple importance shape function...



$$S(\mathbf{r}) \simeq I(\mathbf{r}) \simeq \cos\left(\frac{\pi z}{H_e}\right) J_0\left(\frac{2.405 r}{R_e}\right)$$

- One group diffusion in reflected cylinder
- Zero radial velocity and uniform axial velocity
- Complete mixing in Pump/HEX
- No turbulent or laminar precursors diffusion



Simulation tools – OpenFOAM

Solving the forward and adjoint eigenvalue neutron diffusion problem, with precursors transport...

Forward problem

$$\begin{aligned} \nabla D_g \nabla \phi_g - \Sigma_{a,g} \phi_g - \sum_{g' \neq g} \Sigma_{s,gg'} \phi_g + \sum_{g' \neq g} \Sigma_{s,g'g} \phi_{g'} + \\ + (1 - \beta_0) \chi_{p,g} \sum_{g'=1}^6 \frac{1}{k_{eff}} (\nu \Sigma_f)_{g'} \phi_{g'} + \sum_{i=1}^8 \chi_{d,g} \lambda_i c_i = 0 \end{aligned}$$

$$-\nabla (\mathbf{u} c_i) + \nabla \frac{\nu_T}{S_{CT}} \nabla c_i - \lambda_i c_i + \beta_{0,i} \sum_{g=1}^6 \frac{1}{k_{eff}} (\nu \Sigma_f)_g \phi_g = 0$$



Simulation tools – OpenFOAM

Solving the forward and adjoint eigenvalue neutron diffusion problem, with precursors transport...

Adjoint problem

$$\nabla D_g \nabla \phi_g^* - \Sigma_{a,g} \phi_g^* + \sum_{g' \neq g} \Sigma_{s,gg'} \phi_g^* - \sum_{g' \neq g} \Sigma_{s,g'g} \phi_{g'}^* +$$

$$+ (1 - \beta_0) \frac{1}{k_{eff}} (\nu \Sigma_f)_g \cdot \sum_{g'=1}^6 \chi_{p,g'} \phi_{g'}^* + \frac{1}{k_{eff}} (\nu \Sigma_f)_g \cdot \sum_{i=1}^8 \beta_{0,i} c_i^* = 0$$

$$-\nabla(-\mathbf{u}c_i^*) + \nabla \frac{\nu T}{S_{CT}} \nabla c_i^* - \lambda_i c_i^* + \lambda_i \sum_{g=1}^6 \chi_{d,g} \phi_g^* = 0$$



Simulation tools – OpenFOAM

Solving the forward and adjoint eigenvalue neutron diffusion problem, with precursors transport...

Code snippet – Multi-group neutron diffusion

```
solve
(
  - blockFvm::laplacian(xs->D(), flu)
  + blockFvm::Sp(xs->sigma_a() - xs->sigma_s(), flu)
  ==
  (1/k_eff) * (1 - beta_tot) * ((xs->chi_p() * (xs->nu_tot() &
    xs->sigma_f())) & flu)
  + (xs->chi_d() * delayedNeutronSource)
);

solve
(
  - blockFvm::laplacian(xs->D(), flu_adj)
  + blockFvm::Sp(xs->sigma_a() - xs->sigma_s().T(), flu_adj)
  ==
  (1/k_eff_adj) * (1 - beta_tot) * (((xs->nu_tot() & xs->sigma_f()) *
    xs->chi_p()) & flu_adj)
  + (1/k_eff_adj) * ((xs->nu_tot() & xs->sigma_f()) * adjointPrecursorsSource
);
```



Simulation tools – OpenFOAM

Solving the forward and adjoint eigenvalue neutron diffusion problem, with precursors transport...

Code snippet – Precursors transport

```
solve
(
    fvm::div(phi, prec1)
  - fvm::laplacian(turbulence->nut()/Sct, prec1)
  + fvm::Sp(lam1, prec1)
  - ((xs->nu_tot() & xs->sigma_f()) & flu) * beta1 * (1/k_eff)
);

solve
(
    fvm::div(-phi, prec1_adj)
  - fvm::laplacian(turbulence->nut()/Sct, prec1_adj)
  + fvm::Sp(lam1, prec1_adj)
  - (xs->chi_d() & flu_adj) * lam1
);
```

Eigenvalue problem solved via power iteration

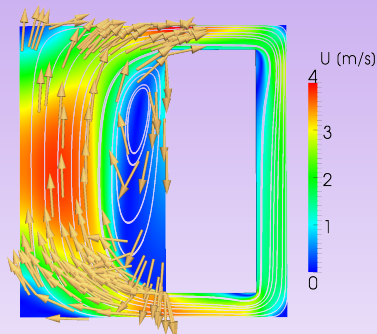


Simulation tools – SERPENT

Transporting DNP inside the Monte Carlo simulation...

When the emission of a delayed neutron is sampled:

- Sample the neutron emission time according to the decay constant
- Transport the precursor until the decay position (Dormand-Prince algorithm)
- Sample the neutron energy



c_i	a_{ij}						
0							
1/5	1/5						
3/10	3/40	9/40					
4/5	44/45	-56/15	32/9				
8/9	19372/6561	-25360/2187	64448/6561	-212/729			
1	9017/3168	-355/33	46732/5247	49/176	-5103/18656		
1	35/384	0	500/1113	125/192	-2187/6784	11/84	
b_i	35/384	0	500/1113	125/192	-2187/6784	11/84	
b_i^*	5179/57600	0	7571/16695	393/640	-92097/339200	187/2100	



Simulation tools – SERPENT

Calculating the effective delayed neutron fraction...

Prompt method is inefficient for β_{eff} and useless for the single $\beta_{eff,i}$ fractions.

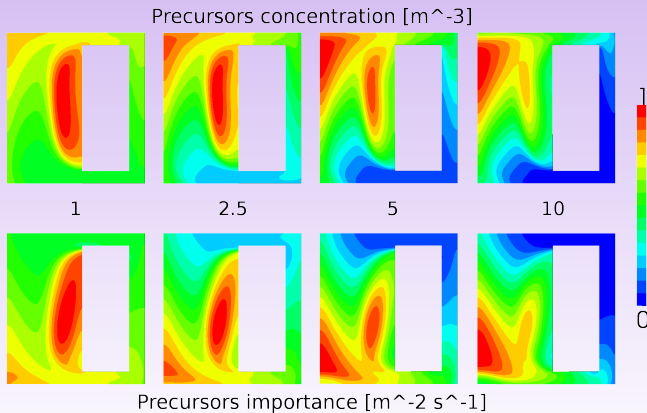
Approximate methods (e.g., van der Mark and Meulekamp) are not suitable due to the presence of high spatial importance effects.

The iterated fission probability is the solution!



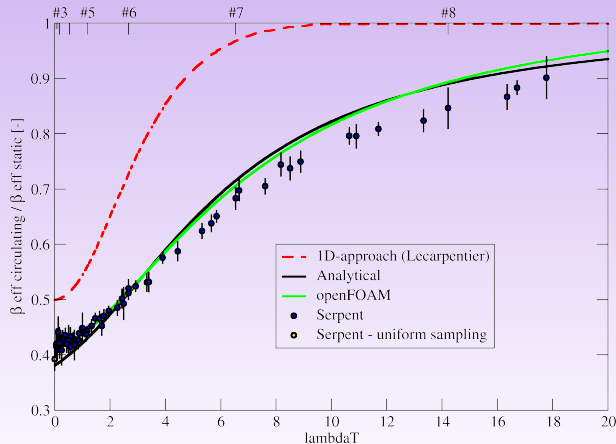
Some results

Precursors concentration and importance, as function of the dimensionless parameter λT (k-epsilon case study)



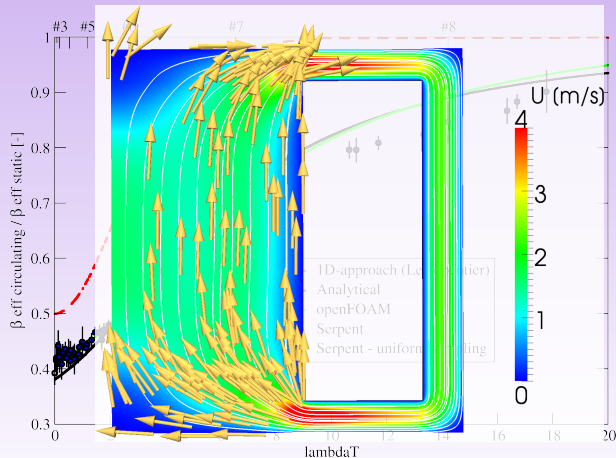
Some results

$\beta_{\text{eff}}^c / \beta_{\text{eff}}^s$ correction factor as function of λT (uniform velocity)



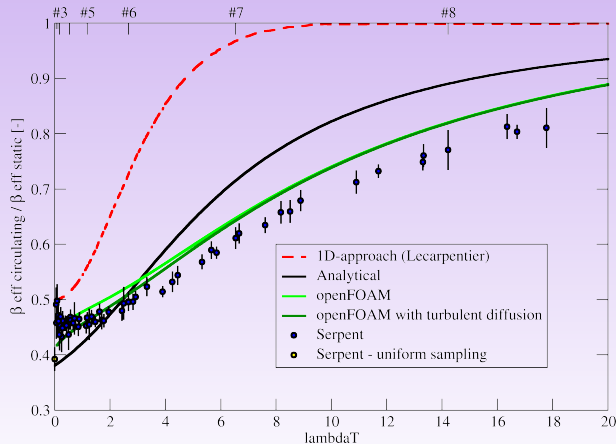
Some results

$\beta_{\text{eff}}^c / \beta_{\text{eff}}^s$ correction factor as function of λT (uniform velocity)



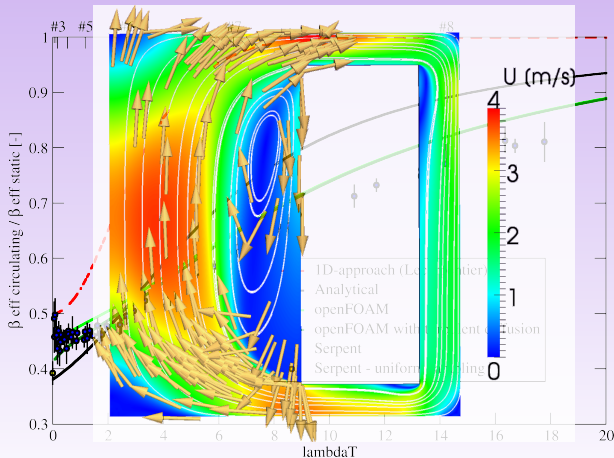
Some results

$\beta_{eff}^c / \beta_{eff}^s$ correction factor as function of λT (k-epsilon)



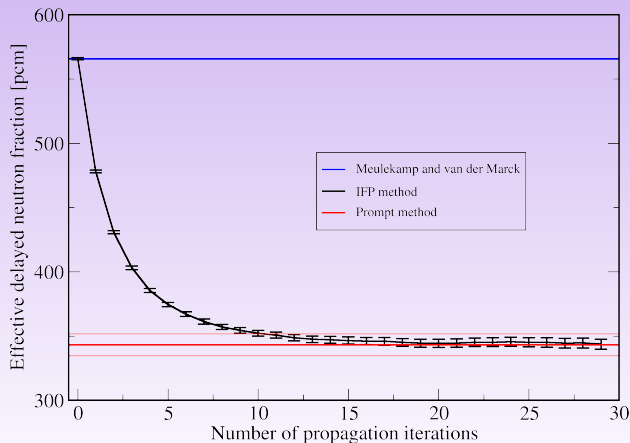
Some results

$\beta_{\text{eff}}^c / \beta_{\text{eff}}^s$ correction factor as function of λT (k-epsilon)



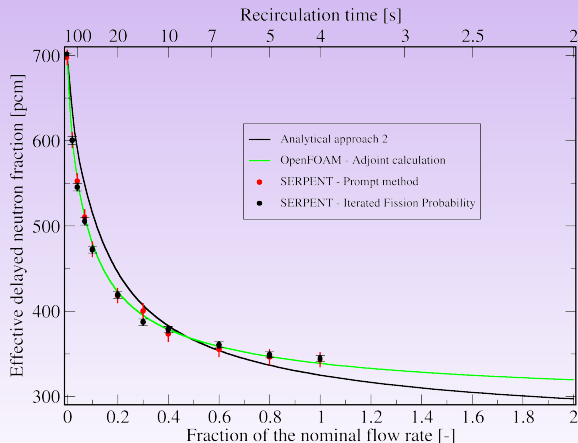
Some results

IFP vs prompt and Meulekamp methods (U^{235} -started, k-eps)



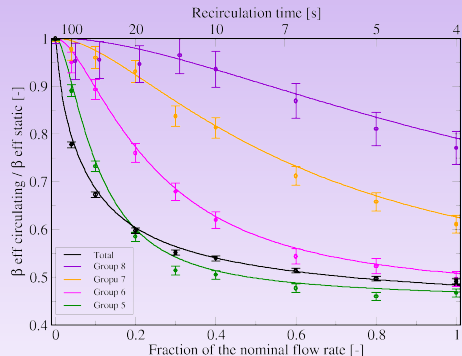
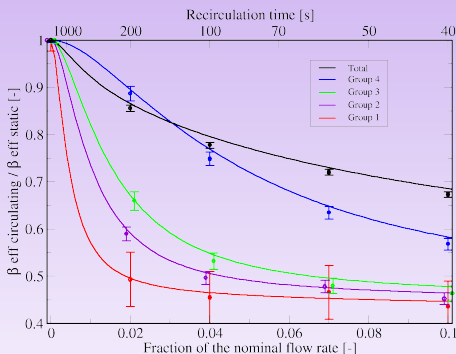
Some results

β_{eff} as function of the flow-rate (U^{235} -started, k-epsilon)



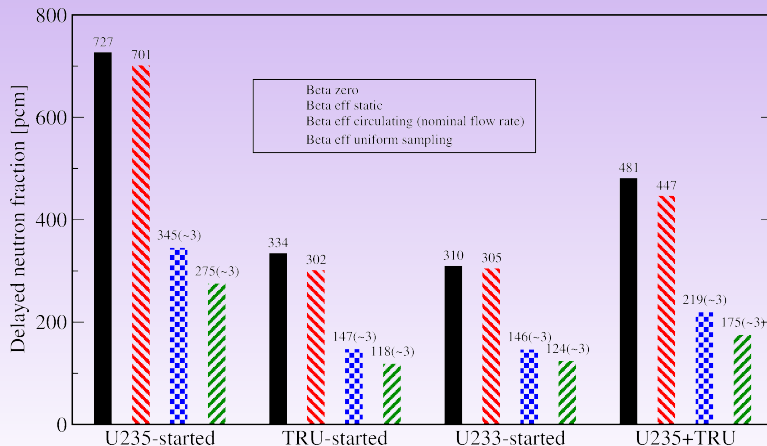
Some results

β_{eff} as function of the flow-rate (U^{235} -started, k-epsilon)



Some results

β_{eff} for different fuel composition



Finite Volume and Delta tracking: two good friends? *

* In collaboration FAST group @PSI (Switzerland).

- Good agreement of β_{eff} between Monte Carlo and multi-group diffusion
- We need reference solution for other multiphysics problems
- We want Monte Carlo solution for complex (real) geometries
Mesh description is easier than combinatorial geometry

Warning Embedding open source C++ FV libraries in Serpent is just one of the possible solutions to be investigated



Finite Volume and Delta tracking: two good friends?

...coupling Serpent and OpenFOAM... what?

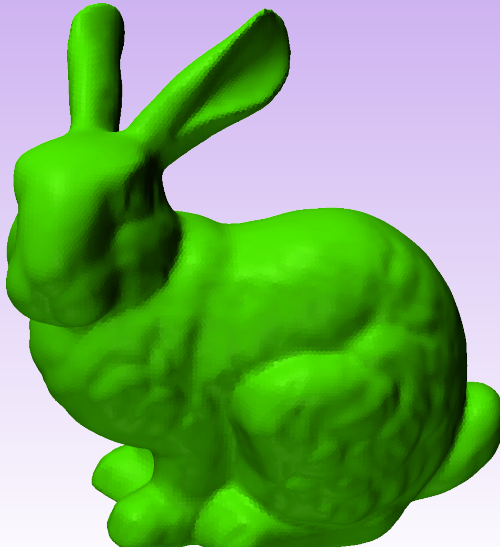
OpenFOAM libraries dynamically linked to Serpent-2

- Serpent takes care of the **hard job**: transporting neutrons
- Serpent “asks” material properties at (X,Y,Z) (e.g., fuel density)
- Serpent “tells” quantities to score at (X,Y,Z) (e.g., fuel density)
- The other physics are solved with standard FV methods
- Coupling is performed at runtime (i.e. every n cycles)
Code-to-code coupling & complex I/O files can be avoided
- The mesh can be deformed at each iteration
- With delta tracking, we just need to know the cell index of (X,Y,Z)
- Fast octree-based mesh search are available in OpenFOAM



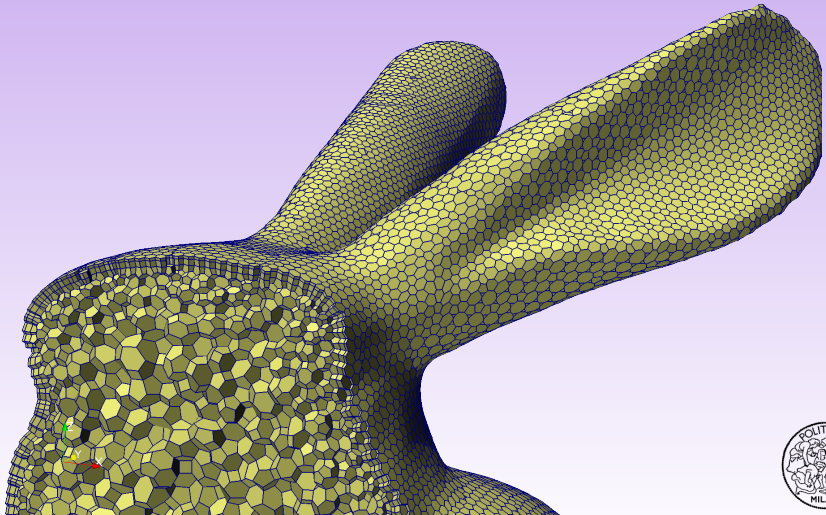
Critical Stanford bunny

Existential question: which is the critical size of a ^{235}U bunny?



Critical Stanford bunny

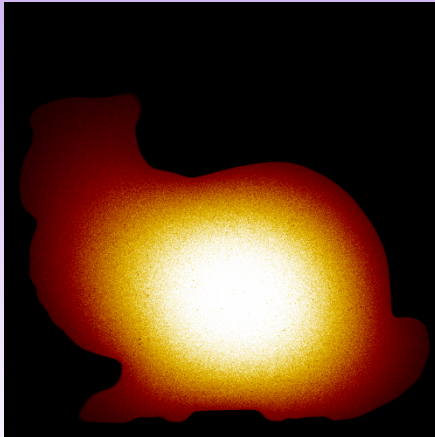
Existential question: which is the critical size of a ^{235}U bunny?



Critical Stanford bunny

Existential question: which is the critical size of a ^{235}U bunny?

Serpent mesh plots at different slices



No animal was harmed during this experiment



Critical Stanford bunny

Existential question: which is the critical size of a ^{235}U bunny?

Main result:

~35% more Uranium with respect to Godiva



Hot Stanford bunny

Dummy multiphysics test case on a bad mesh

Simple multiphysics coupling test case:

- Neutron transport
- Heat diffusion
- Solid mechanics (simple linear-elastic behavior)
- Moving-mesh & material density update

(mass conservation is ensured for each displaced cell)

The small thermal expansions lead to negative feedbacks on neutronics... let's try to see something.

BCs: zero temperature at boundary, no displacement at the center of the bottom base



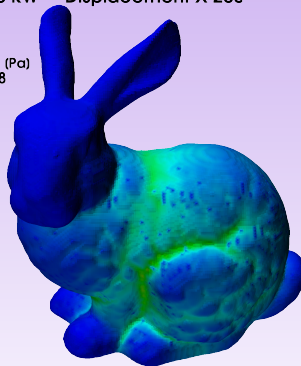
Hot Stanford bunny

Dummy multiphysics test case on a bad mesh

Power: 2.0 kW



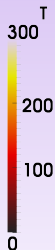
Power: 2.0 kW -- Displacement X 200



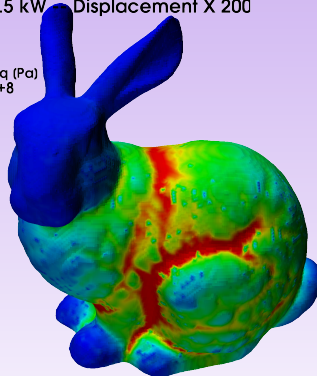
Hot Stanford bunny

Dummy multiphysics test case on a bad mesh

Power: 5.5 kW



Power: 5.5 kW Displacement X 200



Hot Stanford bunny

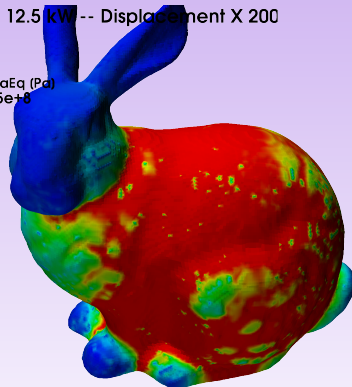
Dummy multiphysics test case on a bad mesh

Power: 12.5 kW



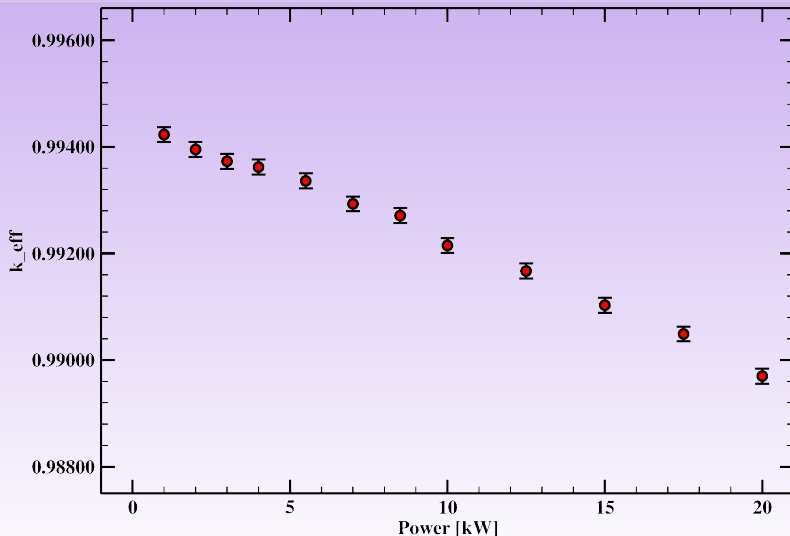
Power: 12.5 kW -- Displacement X 200

sigmaEq (Pa)
 2.5×10^8

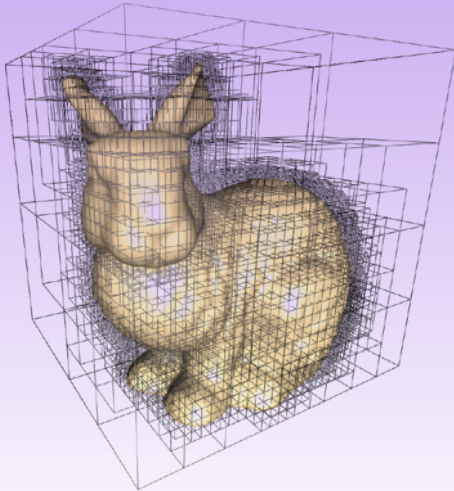


Hot Stanford bunny

Dummy multiphysics test case on a bad mesh



Octree-based mesh search



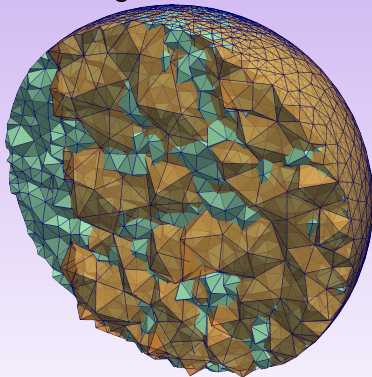
Octree-based mesh search
algorithms available in OF...
room for improvement?

Picture from: [http : //http.developer.nvidia.com/](http://http.developer.nvidia.com/)



Multi-meshes approach

Having the same mesh for everything is often a bad idea.



Different meshes for...

- Scoring energy deposition
- Solving physics (e.g., complex CFD)
- Reading material properties (e.g., density) for delta-tracking

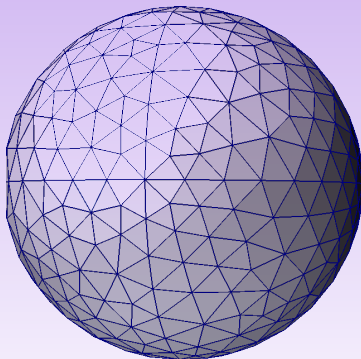
Mesh-to-mesh mapping at runtime

Two mesh searches per collision

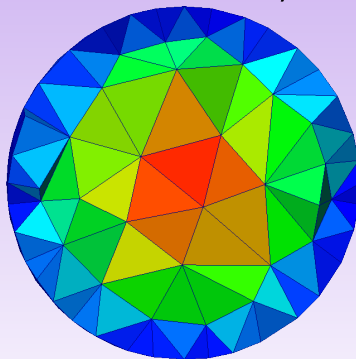


Performances – Godiva test case

Cells: 1758

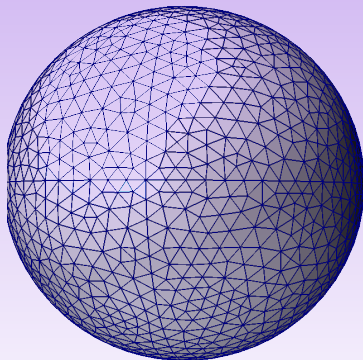


Power density (a.u.)

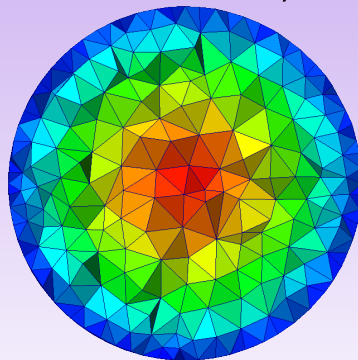


Performances – Godiva test case

Cells: 10840

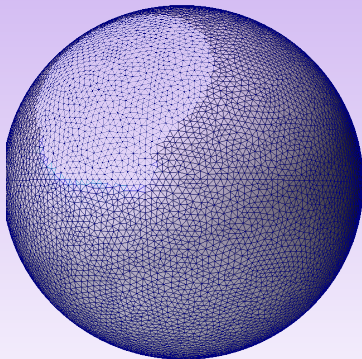


Power density (a.u.)

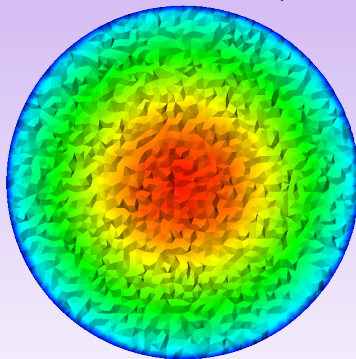


Performances – Godiva test case

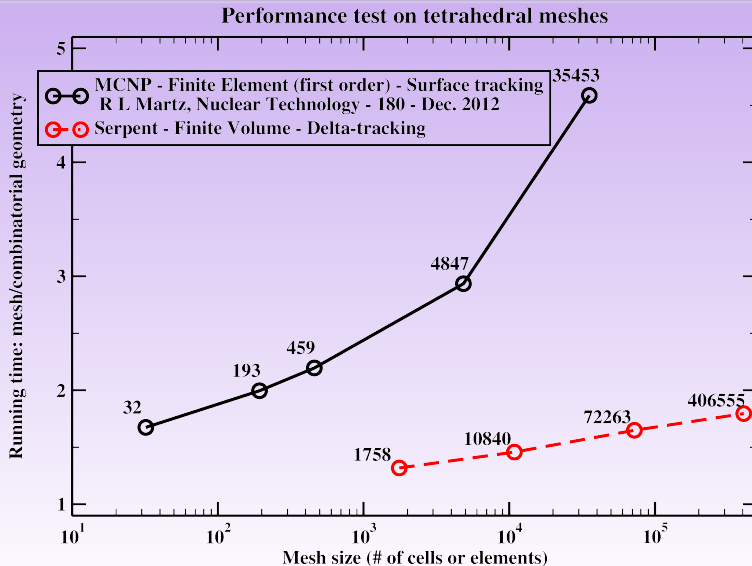
Cells: 406555



Power density (a.u.)

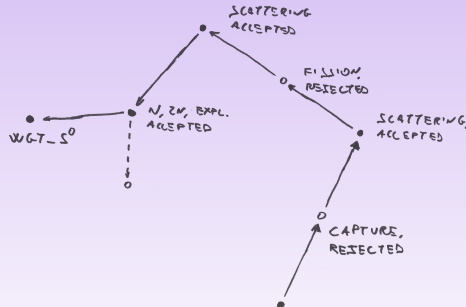


Performances – Godiva test case



Increasing cross-sections & rejecting collisions

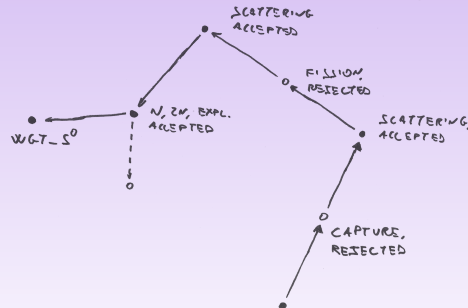
Following a neutron's path



Increasing cross-sections & rejecting collisions

Small cross-sections perturbation

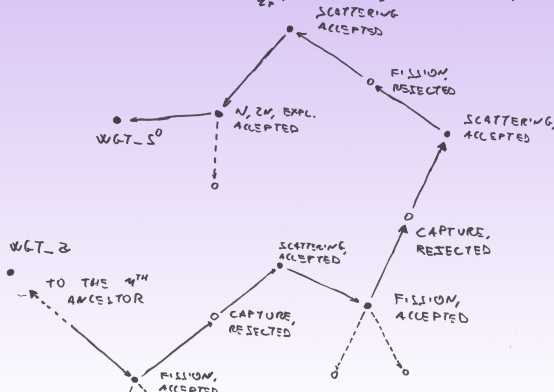
$$WGT-S^* = WGT-S^0 \cdot \left(1 + \frac{\Delta \Sigma_{sc}}{\Sigma_{sc}}\right) \cdot \left(1 + \frac{\Delta \Sigma_s}{\Sigma_s}\right) \cdot \left(1 - \frac{\Delta \Sigma_F}{\Sigma_F}\right) \cdot \left(1 + \frac{\Delta \Sigma_s}{\Sigma_s}\right) \cdot \left(1 - \frac{\Delta \Sigma_c}{\Sigma_c}\right)$$



Increasing cross-sections & rejecting collisions

Adjoint-weighting / fission source redistribution

$$WGT-S^* = WGT-S^0 \cdot \left(1 + \frac{\Delta \Sigma_{sc}}{\Sigma_{sc}}\right) \cdot \left(1 + \frac{\Delta \Sigma_s}{\Sigma_s}\right) \cdot \left(1 - \frac{\Delta \Sigma_f}{\Sigma_f}\right) \cdot \left(1 + \frac{\Delta \Sigma_s}{\Sigma_s}\right) \cdot \left(1 - \frac{\Delta \Sigma_c}{\Sigma_c}\right) \cdot \left(1 + \frac{\Delta \Sigma_f}{\Sigma_f}\right) \cdot \left(1 + \frac{\Delta \Sigma_s}{\Sigma_s}\right) \cdot \left(1 - \frac{\Delta \Sigma_c}{\Sigma_c}\right) \dots$$



Increasing cross-sections & rejecting collisions

We have the perturbed weights, now we need:

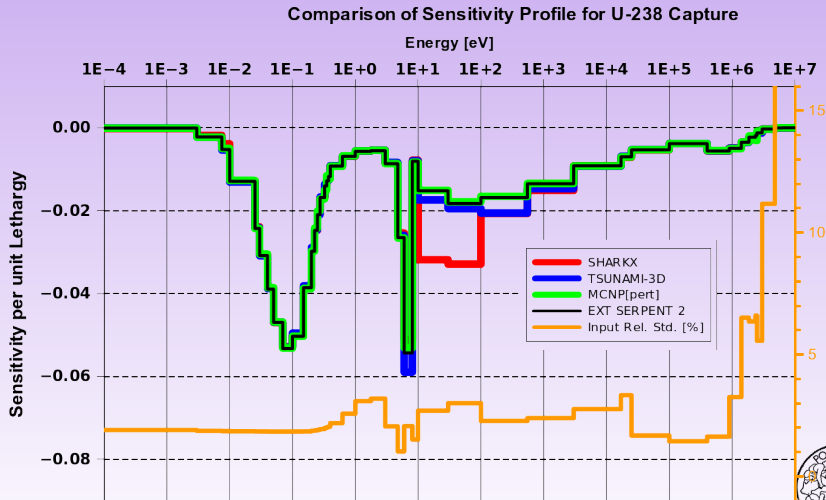
- An unbiased and consistent estimator for $\frac{\Delta k}{k} = f\left(\frac{\Delta \Sigma}{\Sigma}\right)$
- First order expansions around $\Delta \Sigma = 0$
- Keep memory of accepted and REJECTED collisions (also for father, grandfather and so on)
- No need to store all the perturbed weights
Additional required memory does not depend on the number of isotopes, perturbed parameters or energy groups

Boring passages omitted, feel free to ask



First results – PWR pin cell

Comparisons by Mathieu Hursin @PSI

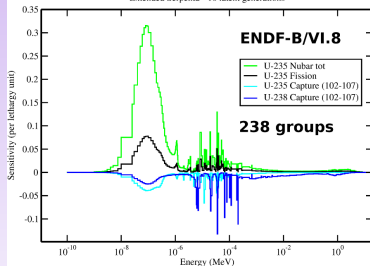


First results – UAM Benchmark

UAM Benchmark – NEA/NSC/DOC(2013)7 – PWR pinCell – TMI-1

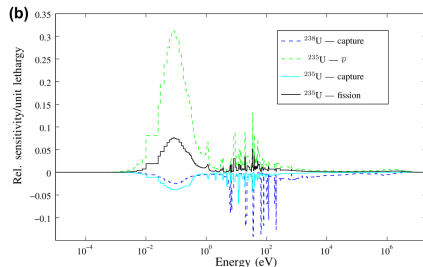
Ext. Serpent-2

PWR pinCell - TMI-1 test case - adj-weighted sensitivity coefficient
Extended Serpent2 - 10 latent generations



TSUNAMI-1D (Maria Pusa)

M. Pusa/Annals of Nuclear Energy 40 (2012) 153–162



First results – UAM Benchmark

UAM Benchmark – NEA/NSC/DOC(2013)7 – PWR pinCell – TMI-1

Nuclide	Parameter	Integral sens. coefficients		
		M. Pusa - Ann. Nucl. Energy 40 153-162		
		CASMO	TSUNAMI	Ext. Serpent-2
U ²³⁸	Σ_c	-0.2609	-0.2219	-0.20201
U ²³⁵	$\bar{\nu}_{tot}$	0.9379	0.9392	0.9390
U ²³⁵	Σ_c	-0.1549	-0.1539	-0.1532
U ²³⁵	Σ_f	0.2559	0.2538	0.2545
U ²³⁸	$\bar{\nu}_{tot}$	0.0621	0.0608	0.0601
Zr	Σ_c	-9.403e-3	-8.315e-3	-8.108e-3
H	Σ_s	0.1952	0.1866	0.1775



First results – UAM Benchmark

UAM Benchmark – NEA/NSC/DOC(2013)7 – PWR pinCell – TMI-1

Looking at the effective delayed neutron fraction as the k-eff sensitivity to $\bar{\nu}_{delayed}$

Parameter	Serpent-2 result
β_{eff} (MEULEKAMP)	723 pcm
β_{eff} (ADJ-WGT IFP - analog)	717 pcm
β_{eff} (ADJ-WGT IFP - implicit)	716 pcm
Sensitivity to $\bar{\nu}_{delayed}$	718 pcm

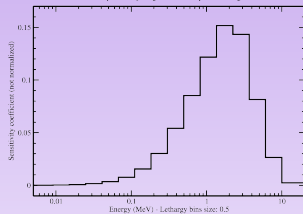


First results – Pu-239 in Jezebel-39

WPEC Subgroup 33 – Document by Sandro Pelloni on OECD-NEA.org

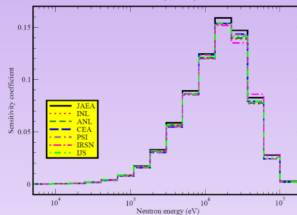
Jezebel (Pu239 configuration) - Pu239 Fission - keff

Extended Serpent2 - adj-weighted sensitivity - 10 latent generations



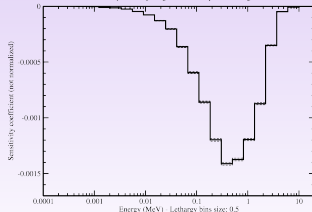
JEZEBEL (Pu-239 configuration)

Pu-239 (n, fission)



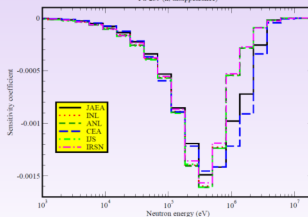
Jezebel (Pu239 configuration) - Pu239 Disappearance - keff

Extended Serpent2 - adj-weighted sensitivity - 10 latent generations



JEZEBEL (Pu-239 configuration)

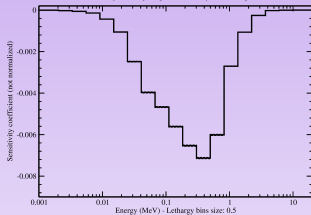
Pu-239 (n, disappearance)



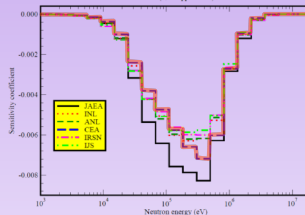
Preliminary results – U-238 in Flatop-39

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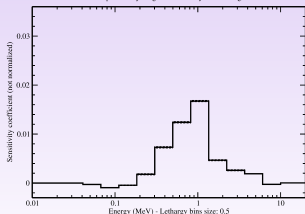
Flatop (Pu239 configuration) - U238 Disappearance - keff
Extended Serpent2 - adj-weighted sensitivity - 10 latent generations



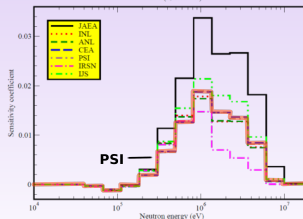
FLATTOP (Pu-239 configuration)
U-238 (n, disappearance)



Flatop (Pu239 configuration) - U238 Inelastic - keff
Extended Serpent2 - adj-weighted sensitivity - 10 latent generations



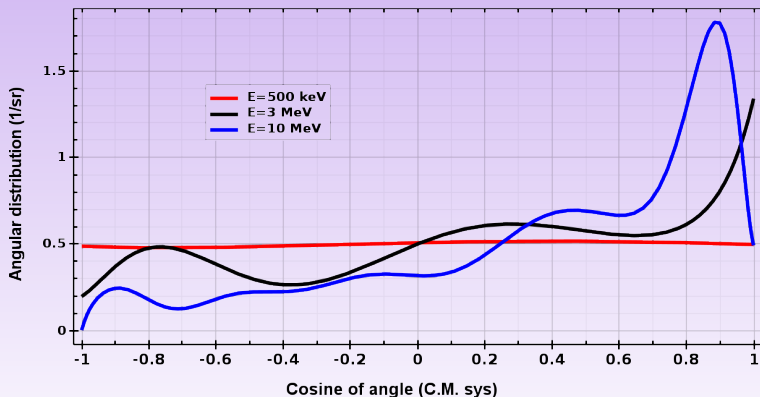
FLATTOP (Pu-239 configuration)
U-238 (n, inelastic)



Preliminary results – U-238 in Flattop-39

WPEC Subgroup 33 – Document by Sandro Pelloni on OECD-NEA.org

Incident neutron data / JEFF-3.1.1 / U238 / MT=51 : (z,n'1)
inelastic scattering to first excited level / Angular distribution



What's next?

- Testing... testing... testing...
(anyone interested?)
- Move to real reactor: Triga reactor of Pavia
(a lot of exp. data and still “cheap” full-core CFD calculations)
- Go back home (Molten Salt Reactors)
- Suggestions?



THANK YOU FOR THE ATTENTION



QUESTIONS? SUGGESTIONS? NEW IDEAS?

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QUESTIONS? SUGGESTIONS? NEW IDEAS?

R. Sanzio et al., La Scuola di Atene, Musei Vaticani, Roma, 1510?.

M. Aufiero et al., *An extended version of the SERPENT-2 code to investigate fuel burn-up and core material evolution of the Molten Salt Fast Reactor*. Journal of Nuclear Materials 441 (2013) 473–486

M. Aufiero et al., *Calculating the effective delayed neutron fraction in the Molten Salt Fast Reactor: analytical, deterministic and Monte Carlo approaches*. Annals of Nuclear Energy. In press.

J. Leppänen et al., *Calculation of effective point kinetics parameters in the Serpent 2 Monte Carlo code*. Annals of Nuclear Energy. Accepted.

M. Aufiero et al., *Development of an OpenFOAM model for the Molten Salt Fast Reactor transient analysis*. To be submitted.