

# **Development of Efficient Improved Core Thermal Hydraulics Predictive Capabilities for Fast Reactors**

***Summary of research and development activities at  
the North Carolina State University***

C. Takasugi, A. Aly, D. Holler, A. Abarca,  
B. Beeler, M. Avramova, K. Ivanov  
North Carolina State University

## Outline

### **1. CTF: Extending Application to SFRs**

- SFR Models and Correlations
- Code-to-Code Comparisons
- Multi-assembly Modelling
- CTF/Dakota Uncertainty Propagation Study

### **2. Hi2Lo Multiphysics Framework**

- CTF CFD-Informed Modelling
- CTF/CTFFuel Thermal Joint Conductance
- NEM Nodal Neutronics Developments
- Thermal Expansion Interfacing

### **3. Conclusions**

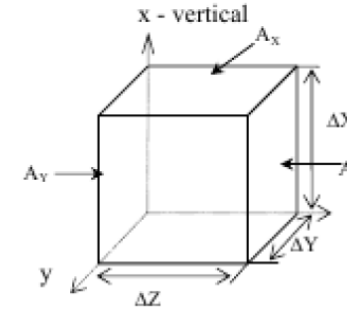
**CTF**

- Developed by the Reactor Dynamics and Fuel Modeling Group (RDFMG) at North Carolina State University (NC SU) in cooperation with Oak Ridge National Laboratory (ORNL).
- Two-fluid, three-field subchannel thermal hydraulics code.

**CTFFuel**

- CTF’s fuel solver, capable of standalone use or interfaced with CTF at the cladding-coolant boundary.
- Used for calculation of thermo-mechanical responses within nuclear fuel rods.

Recent CTF and CTFFuel developments have enabled sodium-cooled fast reactor (SFR) modelling; ongoing work is being done to improve capabilities using high-to-low (Hi2Lo) model informing procedures and integration of SFR capabilities in a newly developed multi-physics platform with the NEM nodal neutronics code.



Mass:

$$\frac{\partial}{\partial t} (\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \vec{V}_k) = L_k + M_e^T$$

Energy:

$$\begin{aligned} & \frac{\partial}{\partial t} (\alpha_k \rho_k h_k) + \nabla \cdot (\alpha_k \rho_k h_k \vec{V}_k) \\ & = -\nabla \cdot [\alpha_k (\vec{Q}_k + \vec{q}_k^T)] + \Gamma_k h_k^i + q_{wk}''' + \alpha_k \frac{\partial P}{\partial t} \end{aligned}$$

Momentum:

$$\begin{aligned} & \frac{\partial}{\partial t} (\alpha_k \rho_k \vec{V}_k) + \frac{\partial}{\partial x} (\alpha_k \rho_k u_k \vec{V}_k) + \frac{\partial}{\partial y} (\alpha_k \rho_k v_k \vec{V}_k) + \frac{\partial}{\partial z} (\alpha_k \rho_k w_k \vec{V}_k) \\ & = \alpha_k \rho_k \vec{g} - \alpha_k \nabla P + \nabla \cdot [\alpha_k (\tau_k^{ij} + T_k^{ij})] + \vec{M}_k^L + \vec{M}_k^d + \vec{M}_k^T \end{aligned}$$

### Sodium Coolant Properties

CTF has implemented liquid sodium properties, however vapor properties were not implemented. CTF must solve two-phases; saturated properties of subcooled liquid sodium are used for the vapor side as a placeholder.

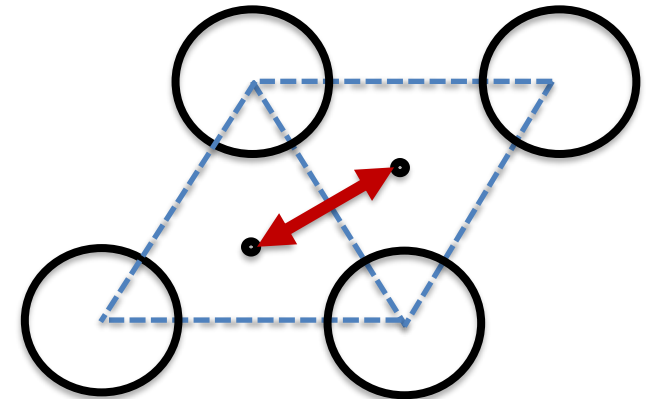
### Gap Heat Conduction

Subchannel-to-subchannel heat conduction was previously neglected in CTF but is more significant for SFRs. The “gap” conduction implemented in CTF dependent on the distance between subchannel centers and a geometry shape factor:

$$q'' = \eta \bar{K} \left( \frac{T_i - T_j}{L} \right)$$

$$\eta = \frac{q''_{local}}{q''_{subchannel}} = 0.777 \left( \frac{P}{D} \right) \left( \frac{S}{D} \right)^{-0.263}$$

P – pitch, S – gap width, D – fuel diameter



## Wire Wrap Correlations

Cheng and Todreas correlations for hexagonal geometry wire-wrapped fuel bundles; few friction factor options including simplified (CTS), detailed (CTD) and upgraded (UCTS and UCTD); distinguish three subchannel types (interior/edge/corner). The mixing correlation considers an effective eddy diffusivity for interior subchannels and a swirl mixing in edge and corner subchannels, induced by the wire wrap, and was implemented in CTF's existing flow mixing framework.

### Friction factor

$$\text{Laminar: } f = \frac{C_{fL}}{Re}$$

$$\text{Turbulent: } f = \frac{C_{fT}}{Re^{0.18}}$$

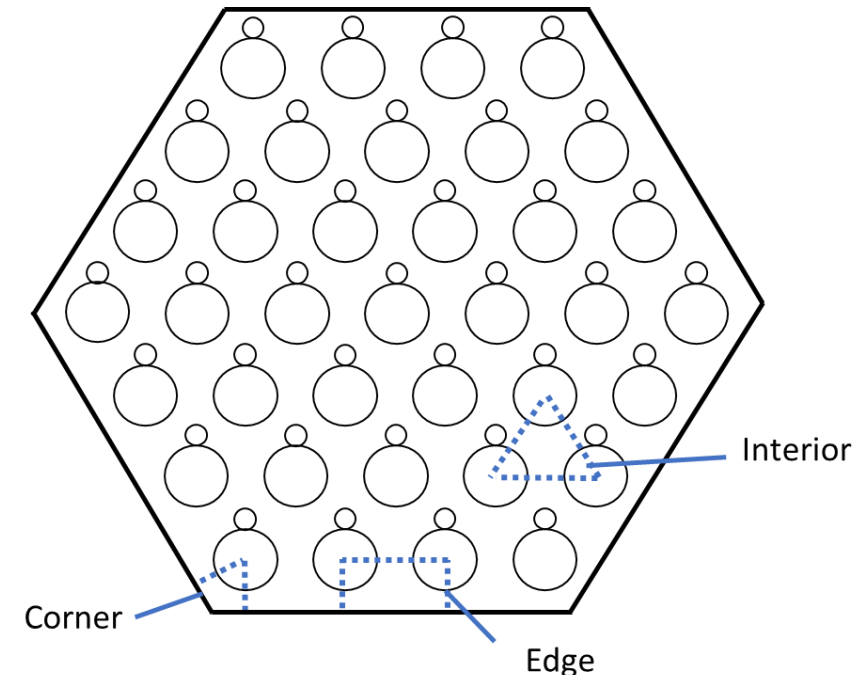
$$\text{Transition: } f = \frac{C_{fL}}{Re} (1 - \psi)^{\frac{1}{3}} + \left( \frac{C_{fT}}{Re^{0.18}} \right) \psi^{\frac{1}{3}}$$

$$\text{Transition (upgraded): } f = \frac{C_{fL}}{Re} (1 - \psi)^{\frac{1}{3}} (1 - \psi^7) + \left( \frac{C_{fT}}{Re^{0.18}} \right) \psi^{\frac{1}{3}}$$

### Mixing parameter

$$\text{Interior: } \epsilon^* = C_m \left( \frac{Ar_1}{A'_1} \right)^{\frac{1}{2}} \tan(\theta)$$

$$\text{Edge/Corner: } C_{1L} = C_s \left( \frac{Ar_2}{A'_2} \right)^{\frac{1}{2}} \tan(\theta)$$



S.-K. Cheng and N. Todreas, "Hydrodynamic Models and Correlations for Bare and Wire-Wrapped Hexagonal Rod Bundles-Bundle Friction Factors, Subchannel Friction Factors and Mixing Parameters," Nuclear Engineering and Design, vol. 92, pp. 227-251, 1986.

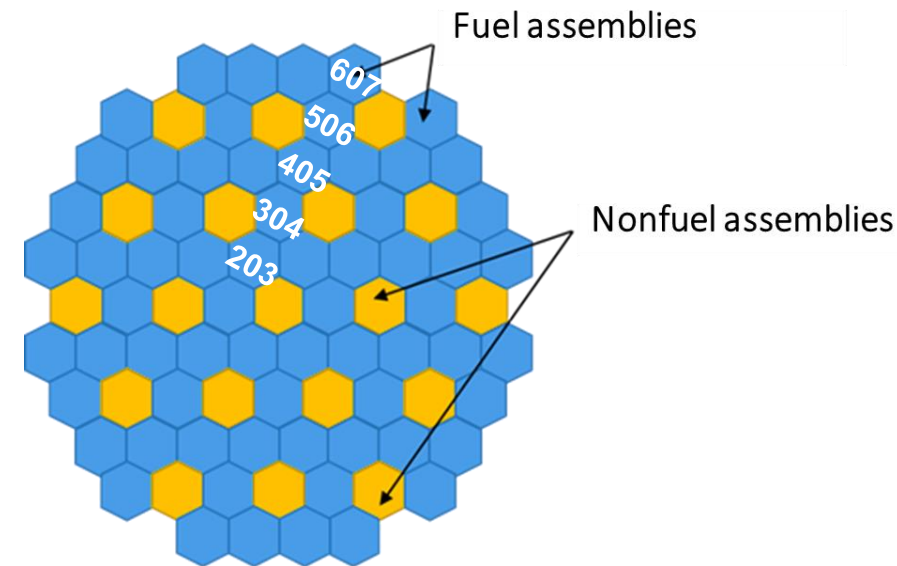
S.-K. Chen, Y. Chen and N. Todreas, "The Upgraded Cheng and Todreas Correlation for Pressure Drop in Hexagonal Wire-wrapped Rod Bundles," Nuclear Engineering and Design, vol. 335, pp. 356-373, 2018.

**Code-to-Code Comparisons with Versatile Test Reactor (VTR) Assembly Models**

- 300 MW<sub>th</sub> SFR design including fuel driver assemblies, test locations and control assemblies.
- Specifications shown are from an SFR model loosely based on VTR scoping studies\*.

CTF modelling of VTR fuel assemblies as confirmatory analysis to SE2-ANL, developed by Argonne National Laboratory, and code-to-code comparison with STAR-CCM+:

- Driver fuel assemblies 203, 304, 405, 506, 607 modeled.
- Power profiles provided by DIF3D.
- Both CTF and SE2-ANL model the full bundle length; STAR-CCM+ case only considered only the active fuel axial length.

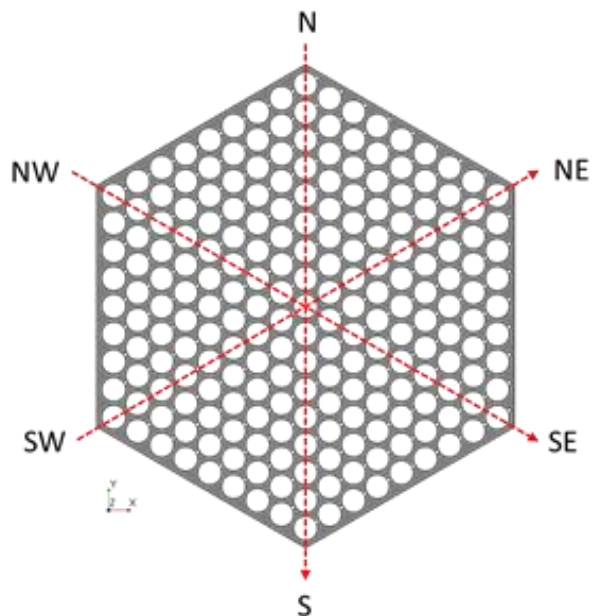


Duct inside flat-to-flat (cm)	11.1
Pins per assembly	217
Pin diameter (cm)	0.625
Clad thickness (cm)	0.045
Wire-wrap diameter (cm)	0.110
Heated length (cm)	80

Fuel Bundle	Power (MW)	Mass Flow Rate (kg/s)	Power-to-Flow Ratio (J/kg)	Inlet Temperature (°C)
203	6.40	33.44	1.914E+05	350
304	5.99	31.27	1.916E+05	350
405	5.18	27.03	1.916E+05	350
506	4.12	21.49	1.918E+05	350
607	3.03	15.81	1.916E+05	350

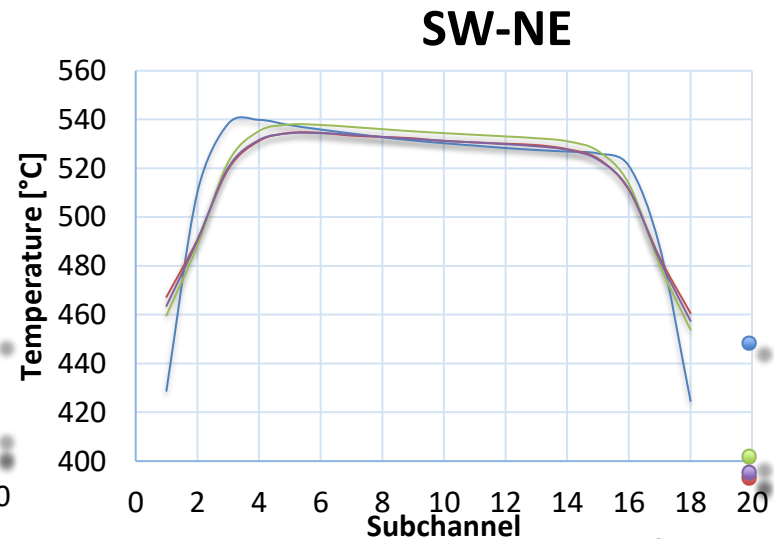
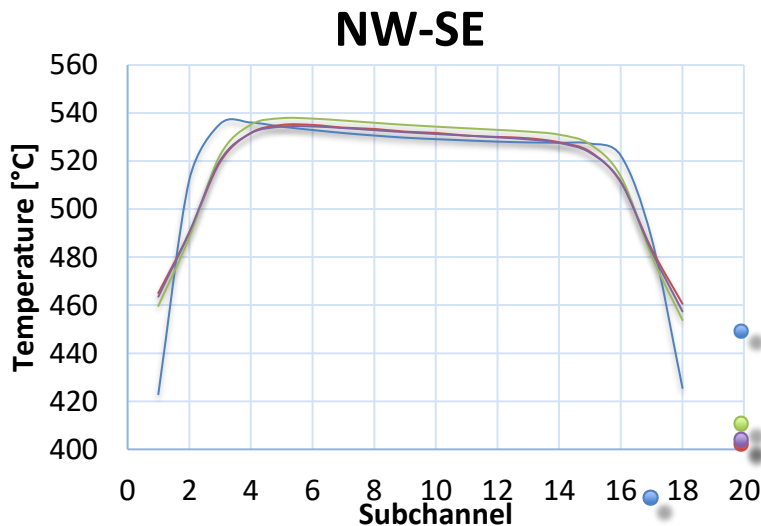
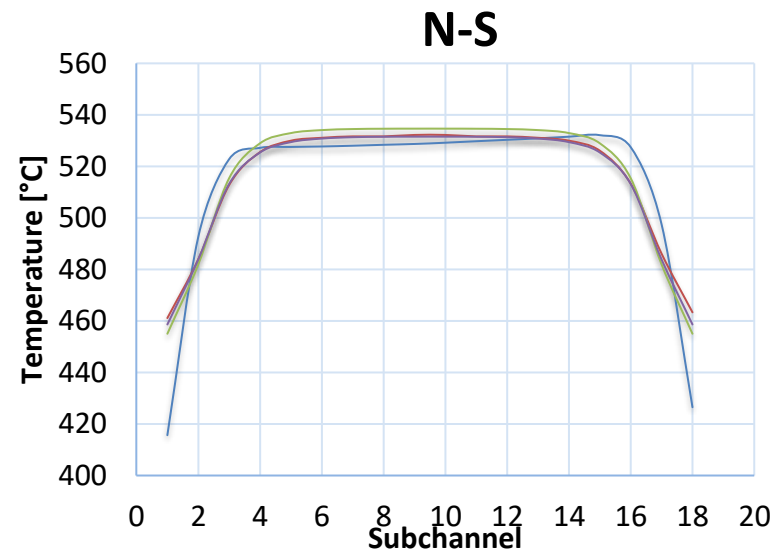
\*A. Abou-Jaoude, S.-J. Yoon, S.E. Bays, "MCNP and CFD Modelling of Sodium Fast Reactor Sub-Assembly Channel to Capture Localized Temperature Peaking," *Proceedings of M&C 2019*, Portland, Oregon, USA, August 25-29, 2019 (2019)

Code-to-Code Comparisons with Versatile Test Reactor (VTR) Assembly Models



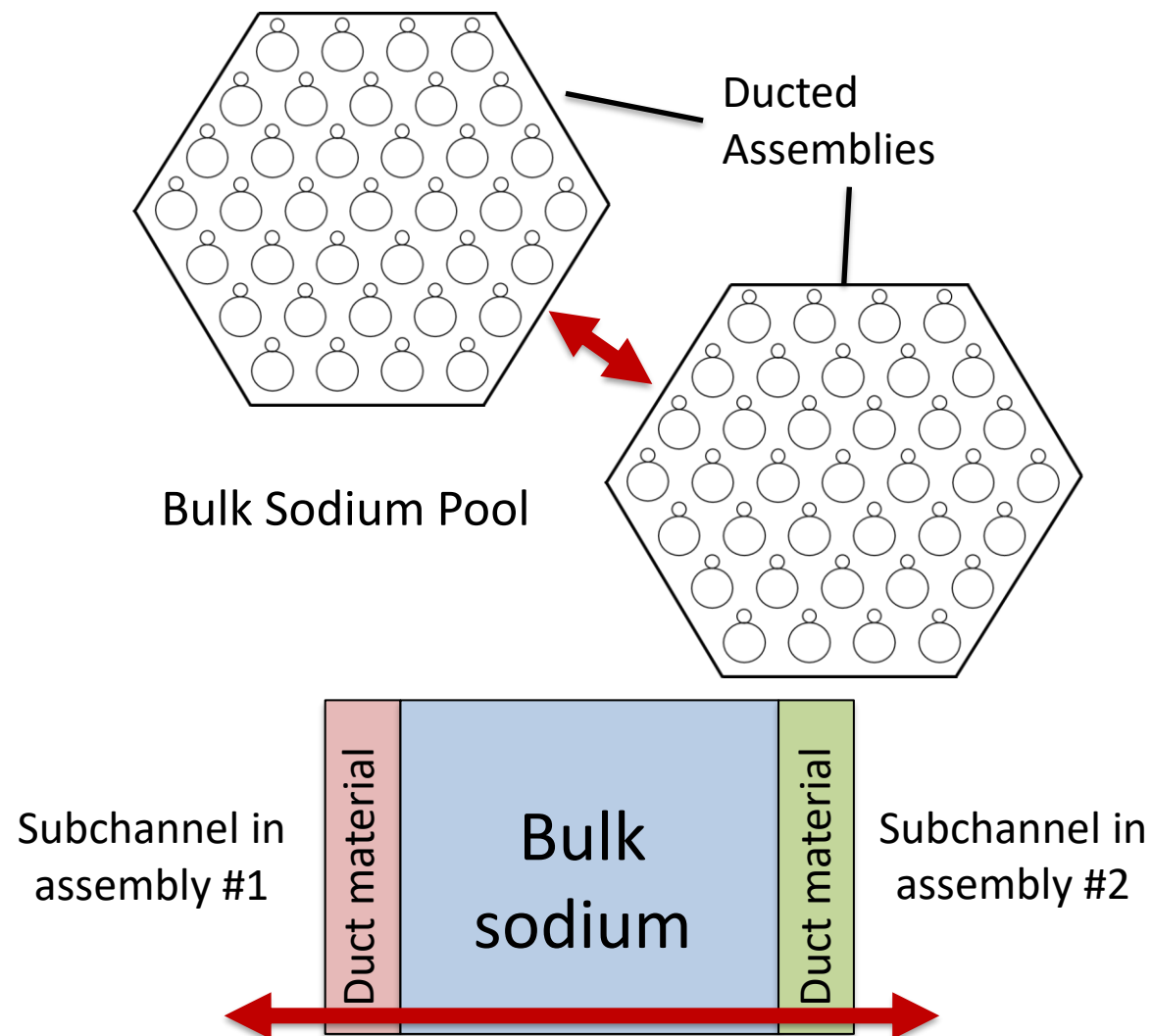
Representative Results Temperature at Top of Active Fuel, Bundle #203

- CFD FA(203) N-S
- SE2 FA(203) N-S
- CTF CTS FA(203) N-S
- CTF CTD FA(203) N-S



### Inter-assembly flow

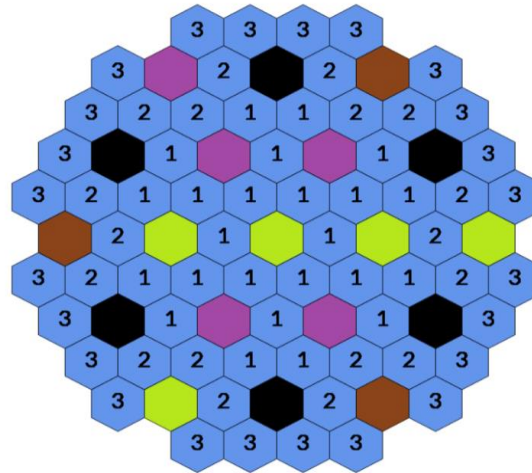
- Bulk sodium subchannels
  - Attempts to equalize pressure loss between all subchannels can restrict convergence without proper selection of inlet mass flows.
  - Separate model applicability.
- Multiple-layer wall heat structure
  - Approximate as duct material, stagnant bulk sodium, duct material layers for heat transfer.
- Initial attempts to model the inter-assembly region focused on the multiple-layer wall option. As the multi-layered wall is not typical to the well-verified LWR capabilities, unexpected erratic behavior that has been repaired and corresponding verification tests incorporated in CTF's testing suite.



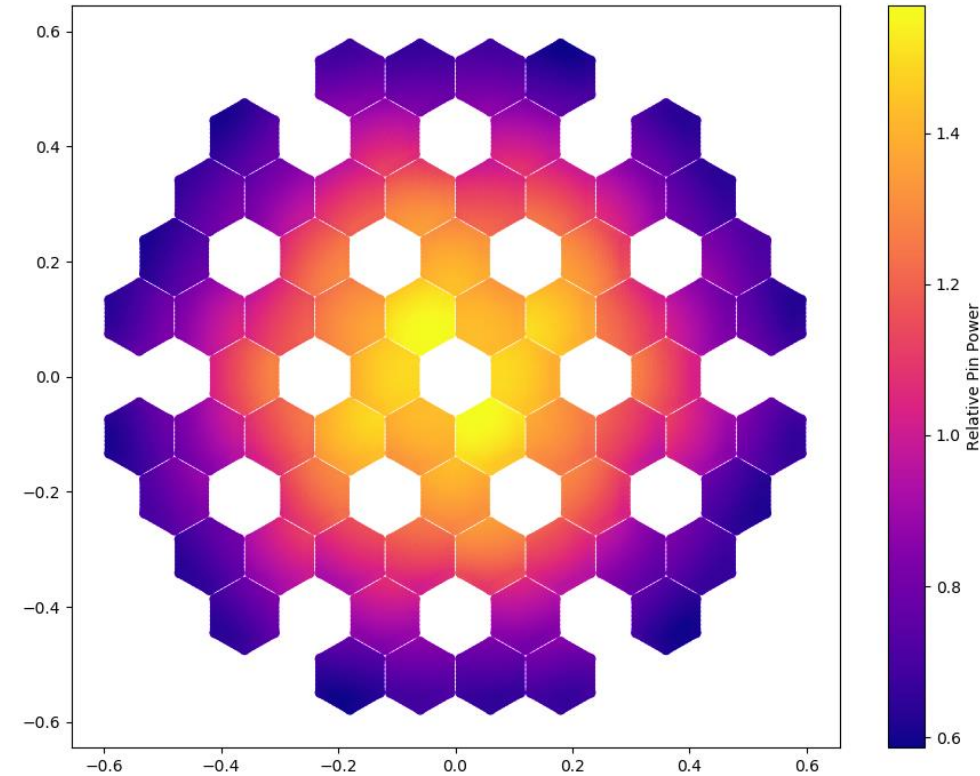


**Extensions for Multi-assembly Models**

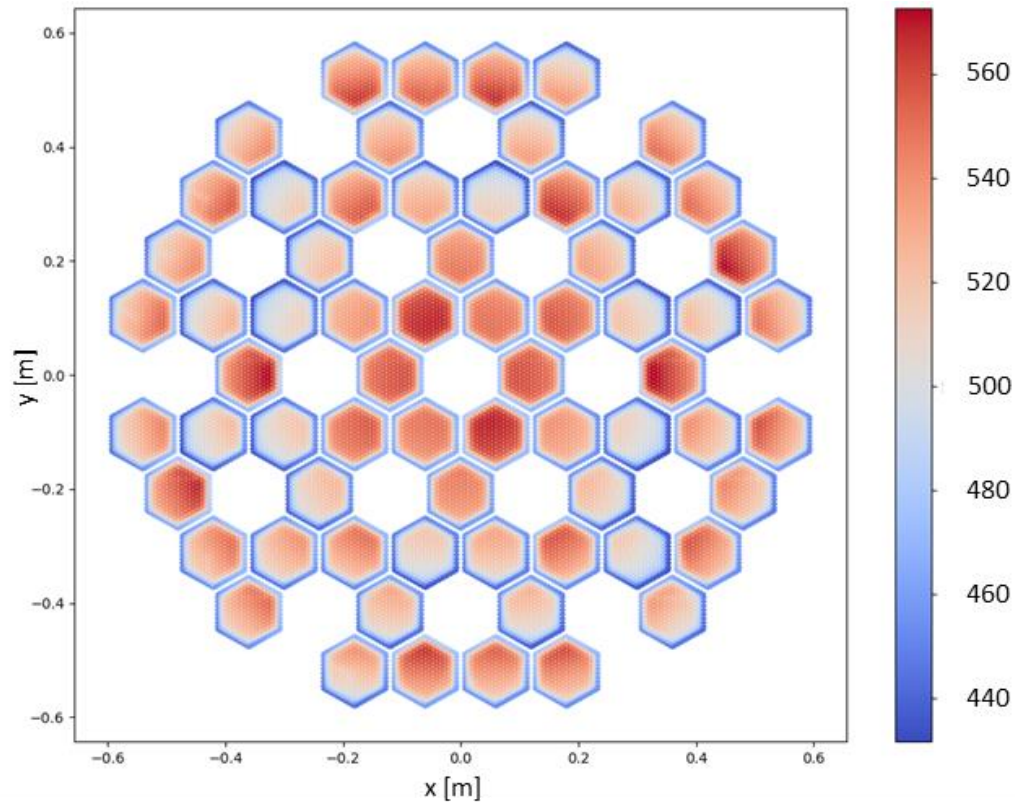
- A CTF model of all VTR driver fuel assemblies was developed with a power profile from Serpent and three core-region inlet mass flow rates.
- Only driver fuel assemblies (of consistent rod/subchannel number) were considered.
- Multi-layer walls linking adjacent fuel bundles for heat transfer.
- Additional modifications to CTF were necessary to permit separate inlet mass flow regions for a parallelized model.



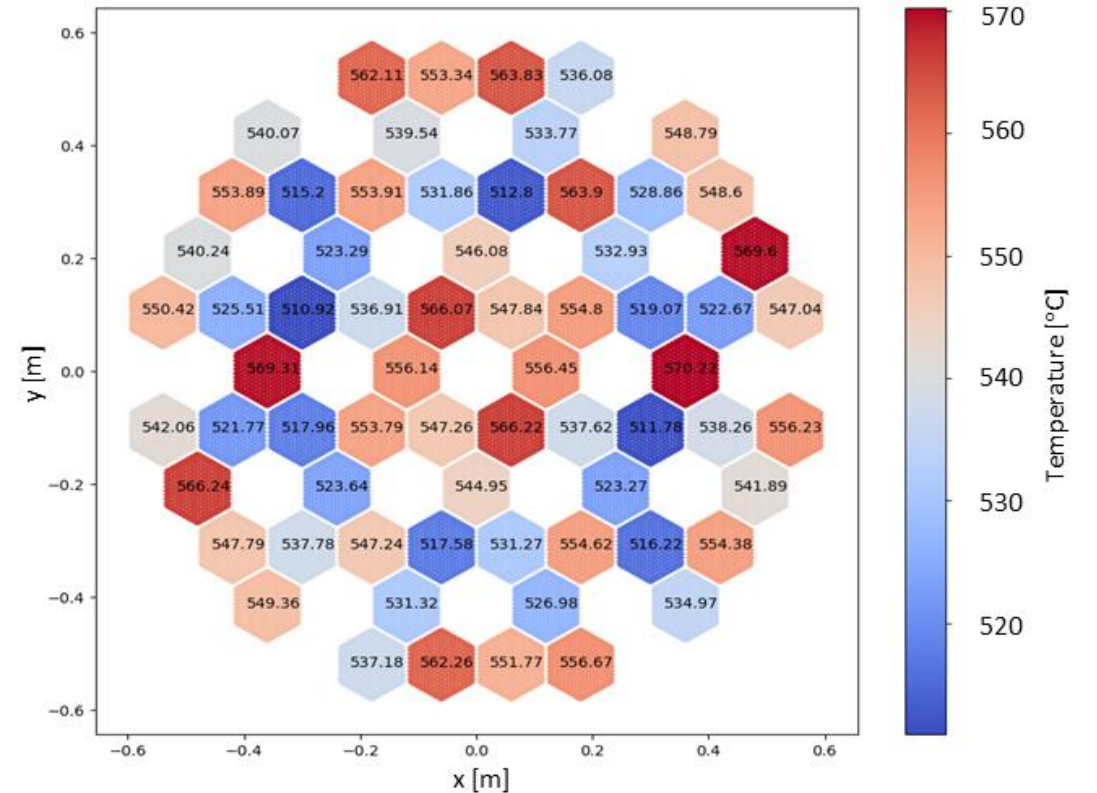
Bundle mass-flow rate  
 1 = 29.8 kg/s  
 2 = 23.2 kg/s  
 3 = 15.9 kg/s



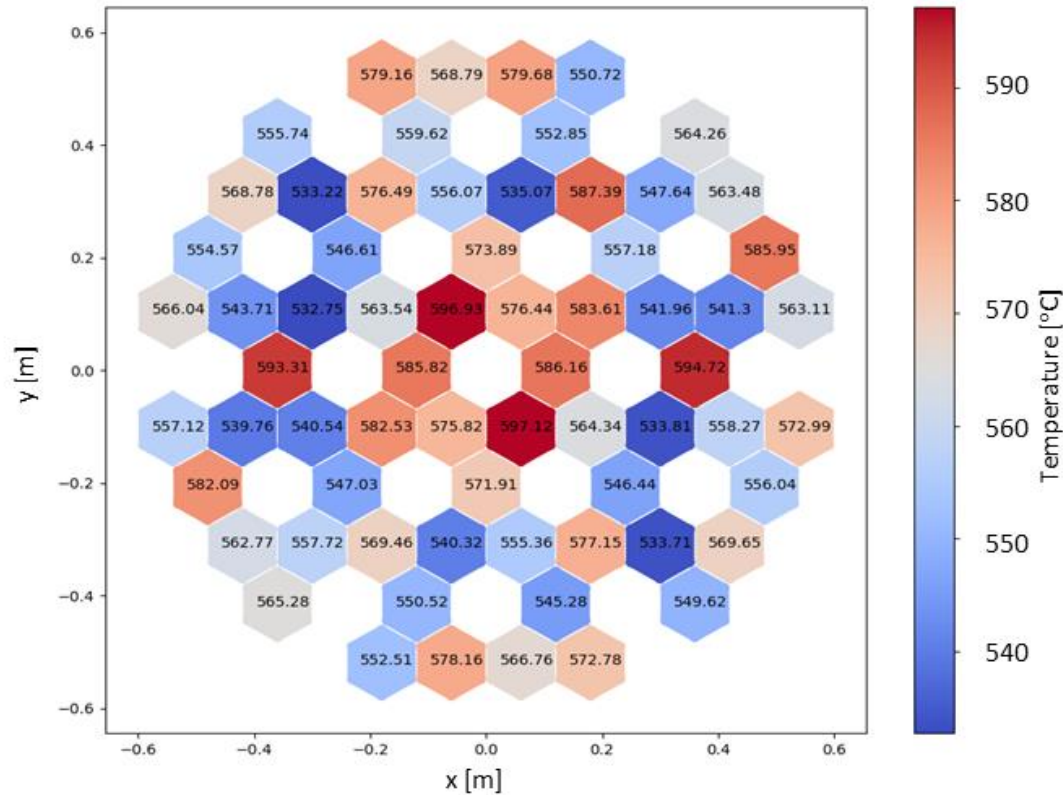
Serpent pin-wise power distribution  
 (individual axial profiles for each bundle)



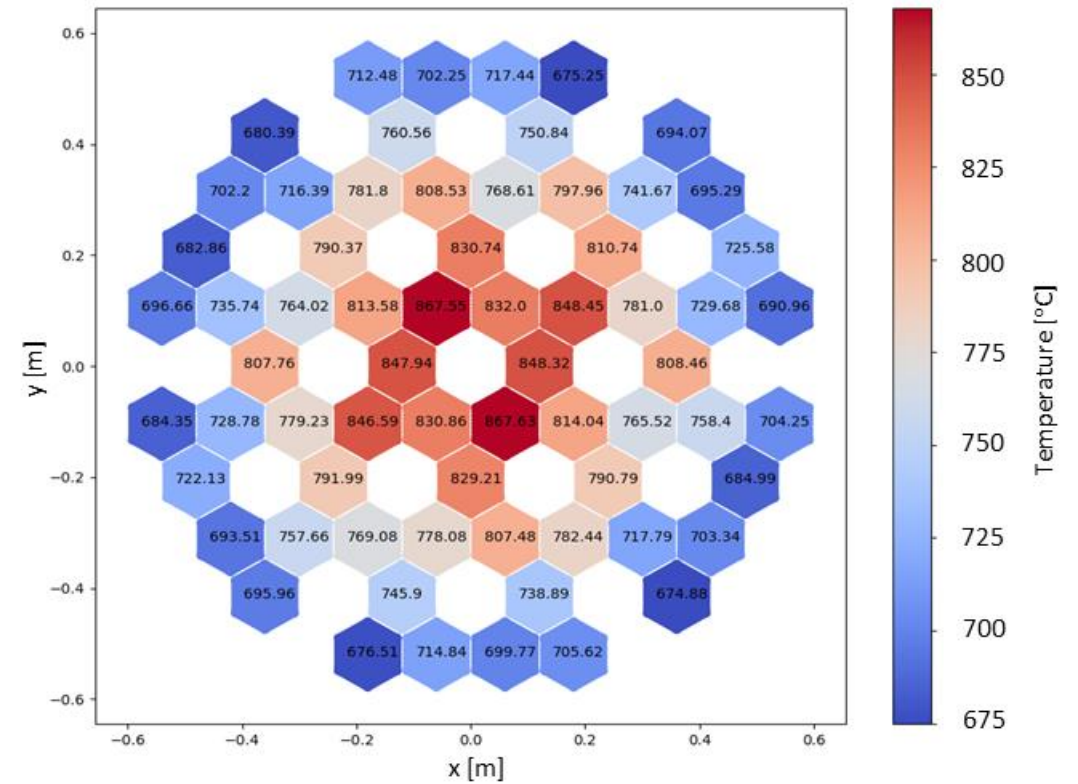
Coolant temperature profile at top of fuel region



Maximum coolant temperature per assembly



Maximum clad temperature per assembly



Maximum fuel-centerline temperature per assembly



### CTF-Dakota Uncertainty Framework

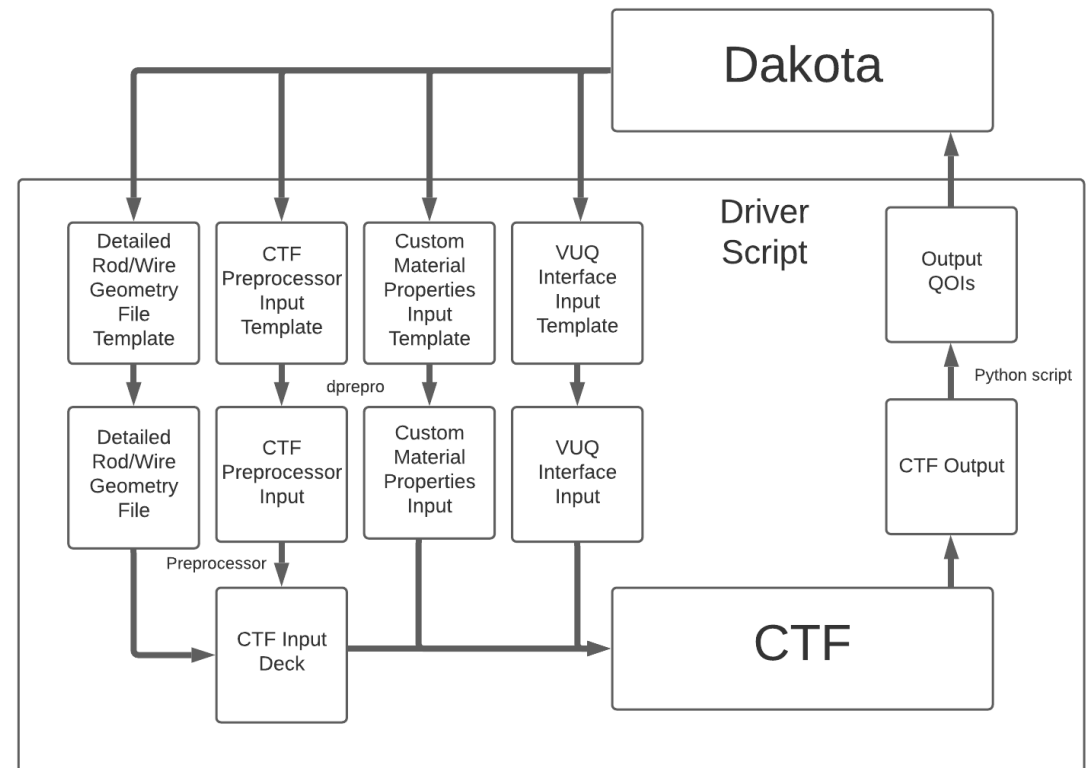
Preliminary Evaluation of the NEA OECD/US NRC Liquid Metal Fast Reactor Core Thermal-Hydraulics Benchmark for Verification, Validation and Uncertainty Quantification for Subchannel and Computational Fluid Dynamics Codes Phase I; modelling of the Texas A&M University (TAMU) 61-pin LMFR Test Facility\* – an unheated, 61-pin mockup of a wire wrapped fuel bundle geometry with p-cymene as the working fluid for flow characterization experiments. The quantity of interest in this evaluation was the pressure drop.

Sources of uncertainty applicable to CTF include:

- rod/wire/bundle geometry
- p-cymene fluid properties (density/viscosity)
- system conditions (mass flow rate/pressure/temperature)
- model uncertainty (friction factor, mixing)

Developed to include options for different geometry sampling assumptions at three mass flow rates:

- Uniform geometry without rod displacement.
- Uniform geometry with rod displacement.
- Independent geometry with rod displacement.



Holler, D., Avramova, M., Takasugi, C., Vaghetto, R., Hassan, Y., "Phase I Specifications and Preliminary Sensitivity Analyses of the OECD-NRC Liquid Metal Fast Reactor Core Thermal-Hydraulics Benchmark", PHYSOR 2020: Transition to a Scalable Nuclear Future, (Proc. Int. Conf. Cambridge, United Kingdom, 2020), (2020).

### Sensitivity Analyses

Three methods applied for A cases (single geometry sample) including parameter study, MOAT analysis, random sampling correlation coefficients.

Relative sensitives are similar between mass flows (1/2/3) for each method, dominated by:

- Friction factor model, directly relating to the pressure drop.
- Rod diameter, has a large impact on flow area and wetted perimeter for some geometry sampling assumptions.

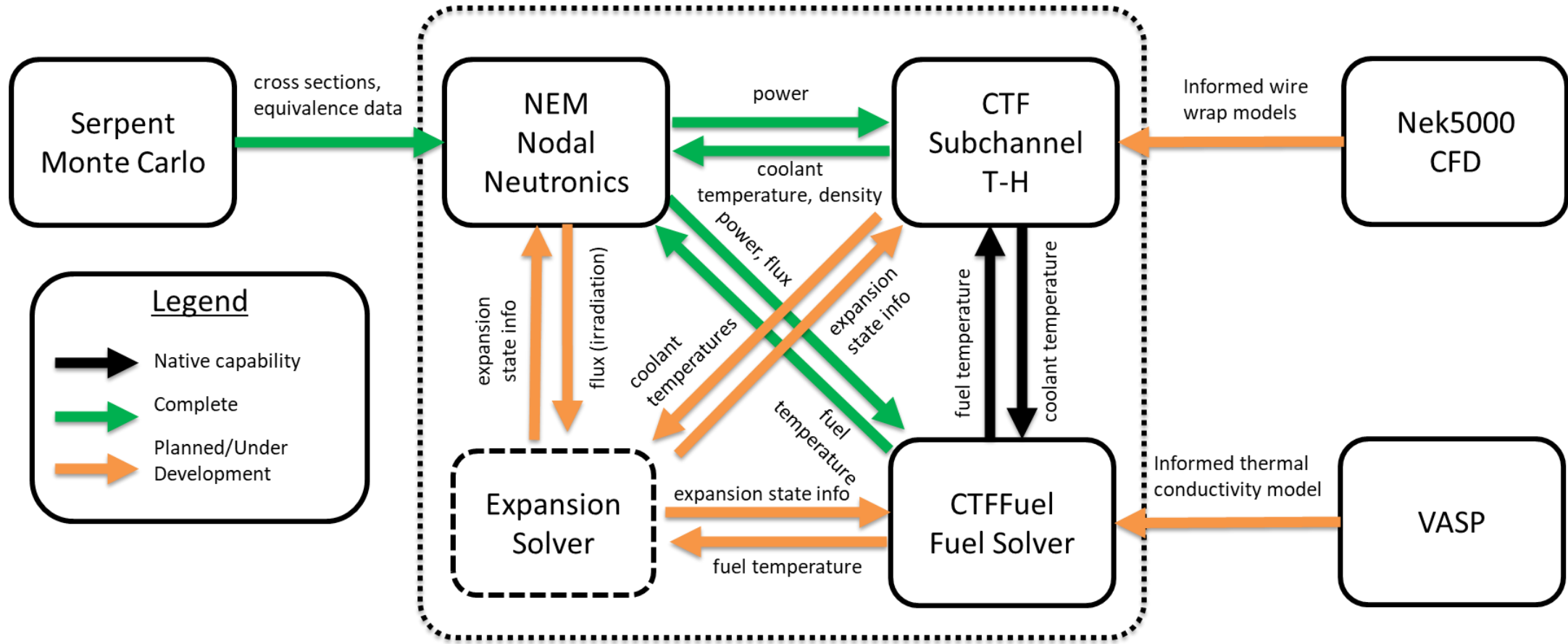
### Uncertainty Estimates

- ‘A’ to ‘B’ differences are impact of rod displacement, which affects flow distribution and channeling.
- Reduced standard deviation in ‘C’ cases expected due to lower impact of geometry on flow area and influence of geometry and model uncertainty (using average values).

PARAMETER	PARAMETER STUDY			MOAT ANALYSIS					
	1A	2A	3A	1A		2A		3A	
	Max $\Delta dP/H$ [%] (t)			$\bar{d}$	$s$	$\bar{d}$	$s$	$\bar{d}$	$s$
Side length	3.6665	2.8105	3.0528	0.8386	0.1927	35.9070	8.6361	274.2000	67.2600
Pin diameter	28.5482	20.8562	21.0417	6.8472	1.4570	246.5900	36.6860	1749.1000	262.2500
Wire diameter	3.9794	2.9514	2.9663	0.5713	0.1300	22.5580	5.3508	160.6400	38.5200
Wire pitch	0.2038	0.7846	0.9644	0.0406	0.0194	9.9858	2.4402	87.0650	20.9300
System pressure	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Inlet mass flow rate	5.3753	5.1053	5.5373	1.2495	0.3081	67.9440	14.1410	522.0300	108.8500
Temperature	2.6076	0.6457	0.2509	0.8146	1.2123	7.9774	2.0613	22.9490	4.8327
Fluid density	0.1789	0.0899	0.0879	0.0414	0.0061	1.1624	0.2412	8.1437	1.7451
Fluid dynamic viscosity	1.9507	0.5048	0.2710	0.4457	0.1473	6.4707	0.8959	24.6840	3.7174
CTD Friction Factor	36.0661	24.0001	23.7903	8.2444	1.1674	312.0100	51.1970	2192.9000	368.3400
CT Mixing	0.0011	0.0071	0.1023	0.0010	0.0009	0.1677	0.0932	9.2273	3.8133

CASE ID	ROD/WIRE SAMPLING	MEAN [Pa]	STANDARD DEVIATION [Pa]	SKEWNESS	KURTOSIS
1A	Synchronized (no displacement)	11.80180	1.95413	0.36381	0.26188
1B	Synchronized (displacement)	11.58692	1.78943	0.22980	0.10272
1C	Independent	11.56968	1.42043	0.01811	-0.19520
2A	Synchronized (no displacement)	649.11381	66.02106	0.21728	0.17967
2B	Synchronized (displacement)	648.66496	66.27508	0.23859	0.14326
2C	Independent	647.17120	52.75335	0.01698	-0.16384
3A	Synchronized (no displacement)	4599.49462	466.87931	0.21884	0.17699
3B	Synchronized (displacement)	4597.16161	468.89133	0.24016	0.14286
3C	Independent	4585.82708	372.74201	0.02283	-0.15371

Hi2Lo Multiphysics Platform for SFR Modelling



## CTF CFD-Informed Modelling

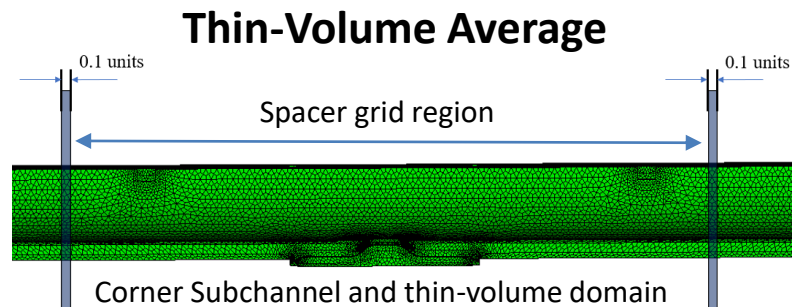
The high-fidelity CFD code Nek5000 has been applied to develop CFD-informed models for CTF. Nek5000 uses the Spectral Element Method (SEM); has incompressible, turbulent flow with LES, DNS and RANS capabilities; and has been used in flow analysis for nuclear engineering applications.

A study has recently applied CFD to investigate informed spacer-grid loss coefficients for CTF LWR modelling\*:

- Inform CTF with total grid loss coefficient data obtained from planar averaging of Nek5000 solution.
- Investigate the accuracy of three planar averaging methods to predict pressure drop across spacer grids for Reynolds numbers 1,000 to 10,000:
  - Thin-volume averaging
  - Averaging with history points
  - VSI postprocessing
- Study repeated for different spacer grid geometries:
  - Mixing vane
  - Non-mixing vane
  - Simplified spacer grid

\*N.A. Kulkarni, D. Holler, M. Avramova, "High-to-Low Informing Schemes for Core Thermal Hydraulics Calculations", Sixth OECD-NEA C5G7-TD Benchmark Meeting (C5G7-TD-6), Aix-en-Provence, France (2022).

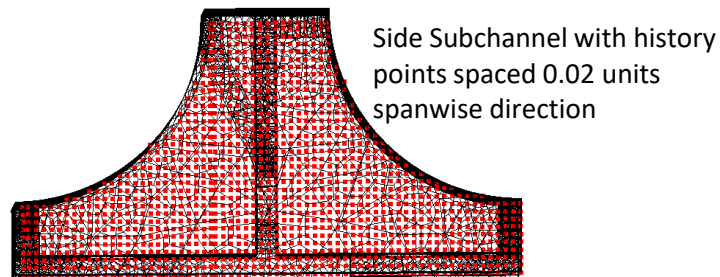
CTF CFD-Informed Modelling



Nodes lying within a thin volume are considered for averaging.

"Dillon Shaver-ANL/usrcode," <https://github.com/dshaver-ANL/usrcode/blob/master/utilities.f>, Github, Inc. (2020, accessed August 3, 2021)

Averaging with History Points



Probe points are placed in the domain for data extraction, arithmetic mean is calculated over each plane.

VisIt Postprocessing

Plane slices are generated at the same locations as other methods for data extraction, arithmetic mean is calculated on pressure data extracted from a plane. VisIt is an open-source visualization utility.

H. Childs, et. al.. "VisIt: An End-User Tool For Visualizing and Analyzing Very Large Data", In "High Performance Visualization - Enabling Extreme-Scale Scientific Insight", First Edition, Chapter 16, pp. 358-396, October 2012, Chapman and Hall/CRC.

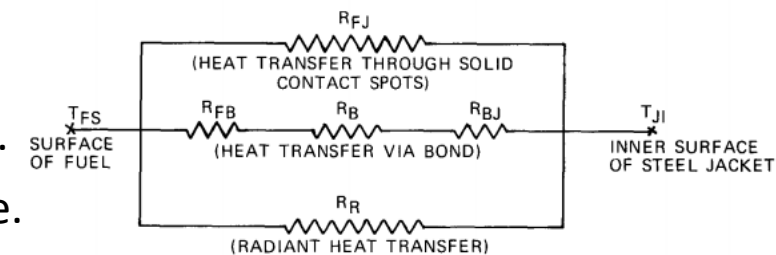
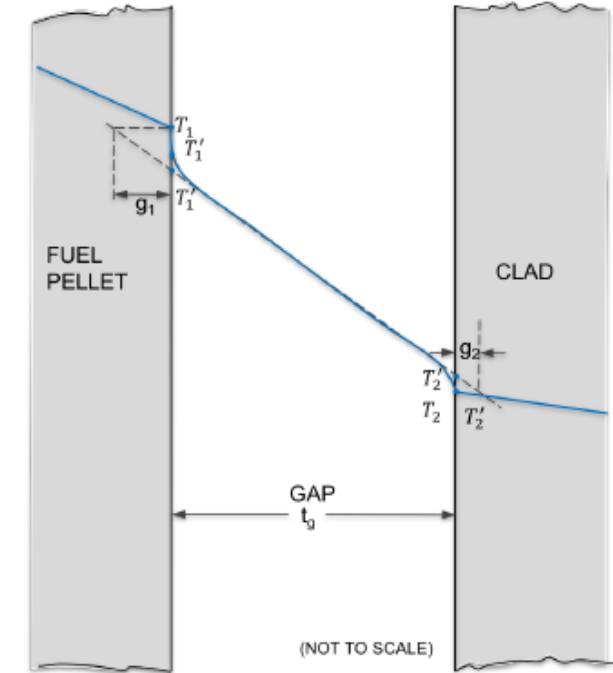
Plans are under development to utilize Nek5000 to develop informed models for CTF's SFR-applications in wire-wrapped geometries. The development of lookup tables for mixing coefficients for wire-wrapped subchannel geometries is planned as a first step of this process.

\*N.A. Kulkarni, D. Holler, M. Avramova, "High-to-Low Informing Schemes for Core Thermal Hydraulics Calculations", Sixth OECD-NEA C5G7-TD Benchmark Meeting (C5G7-TD-6), Aix-en-Provence, France (2022).



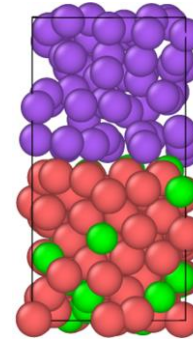
### Thermal Joint Conductance

- The joint thermal conductance across the gap is based on interfacial resistance, resistance to heat transfer through the filling fluid and contact resistance.
- The gap conductance in CTF/CTFFuel is modeled by assuming a jump distance over which a fictitious jump in temperature occur due to incomplete thermal mixing.
- The temperature jump distances are based on empirical models for the specific solid and liquid - current models in CTF/CTFFuel are based on oxide fuel and helium filled gap.
- Metallic U-Zr fuel with a sodium filled gap cannot be modeled in the same way. To accurately model gap conductance, a model is formulated that considers the interfacial thermal conductance at the fuel and the cladding surfaces, thermal conductance through the sodium bond and metal contact conductance for a closed gap.
  - Literature is reviewed for a suitable correlation for the metallic contact conductance.
  - The interfacial thermal conductance is based on the acoustic mismatch theory.
  - Hi2Lo modeling was performed to determine the interfacial thermal resistance.



### Thermal Joint Conductance

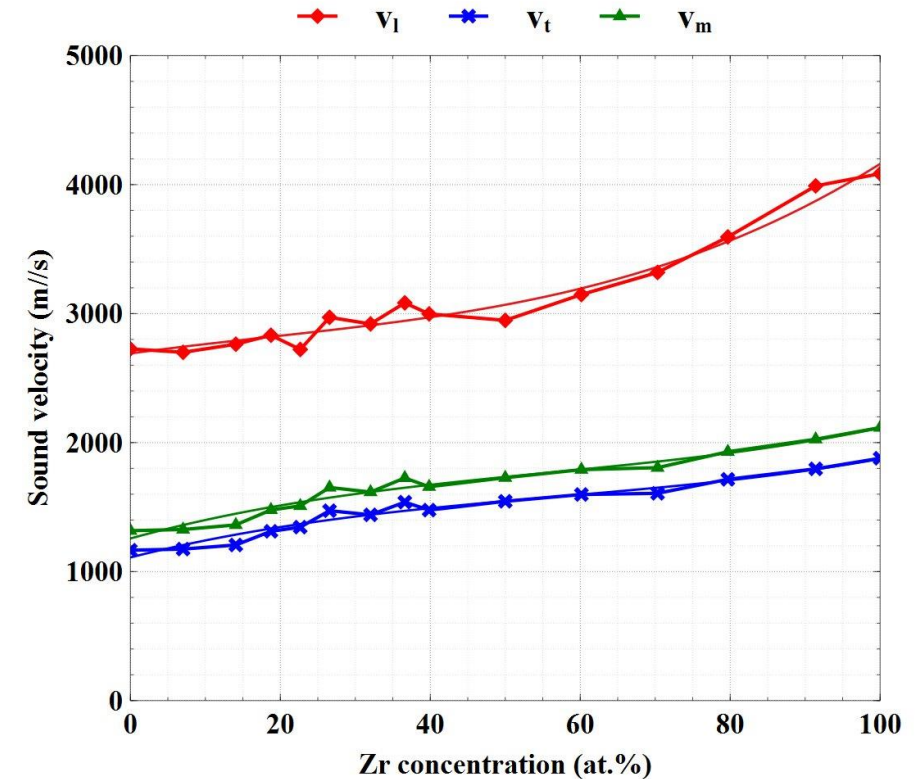
- The Vienna Ab initio Simulation Package (VASP) code was used to perform atomistic modeling of the U-Zr metallic fuel to determine the speed of sound in metallic fuel as a function of zirconium concentration.
- The interfacial energy of the fuel surface was determined, and it was shown that above 1000 K sodium completely wets the fuel surface which enhances the interfacial heat transfer.
- The impedance to the energy transfer between a solid and a liquid is related to the mismatch between the speed of sound and the density of the two media.



$$v_l = \left( \frac{3B + 4G}{3\rho} \right)^{\frac{1}{2}}$$

$$v_t = \left( \frac{G}{\rho} \right)^{\frac{1}{2}}$$

$$v_m = \left( \frac{1}{3} \left( \frac{2}{v_t^3} + \frac{1}{v_l^3} \right)^{-\frac{1}{3}} \right)$$



## Thermal Joint Conductance

- With the determination of the sound velocity in the fuel and the liquid sodium, a model for the interfacial conductance was created:

$$h_I = 6 \frac{nN_A K_B}{M_F} \alpha F \left( \frac{V_F}{V_B}, T \right)$$

- Literature was reviewed for a model of the metal contact conductance and a model by Yovanovich was chosen:

$$\frac{h_c \sigma}{km} = 1.25 \left( \frac{P}{H_c} \right)^{0.95}$$

- The gap conductance was taken as:

$$h_g = \frac{K_{Na}}{t}$$

- The joint thermal contact conductance was taken as a combined function of the following:

$$h_j = f(h_c, h_g, h_I)$$

## NEM

- 3D multigroup nodal diffusion code.
- Developed by the Reactor Dynamics and Fuel Modeling Group (RDFMG) at NCSU.
- Cartesian, Cylindrical, Hexagonal-z geometries.
- Fourth-order quadratic leakage formulation of the Nodal Expansion Method (NEM), utilizing a response matrix solution technique.

Branching developments of the NEM code have been made over the years, with primary development focus being on Cartesian geometry.

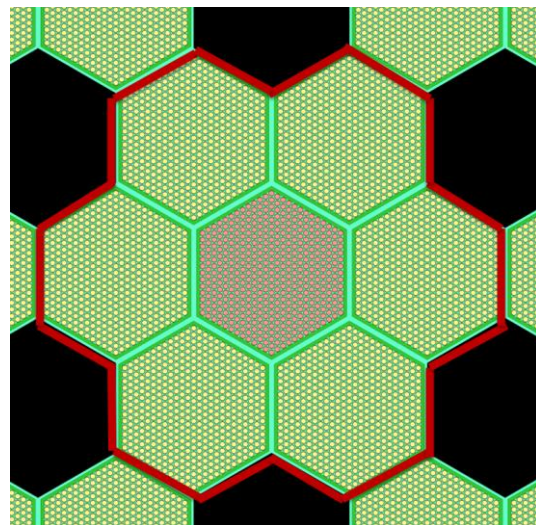
Desire to extend its use for SFRs has led to the current work to restore and further develop the NEM code for Hex-z geometry.

- Redeveloped according to latest documentation and intermediate developments made in Cartesian versions of the code. Code-to-code comparisons have been performed and shown good agreement with codes utilizing similar methodology.
- Implementing a streamlined two-step Serpent/NEM calculation scheme for cross section and discontinuity factor generation.



### 2D DF Test

7 fuel assemblies (2 Compositions),  
reflective boundary conditions



Code	Eigenvalue	Error
Serpent	1.13066	-
NEM-RDFMG without DFs	1.13064	-2 pcm
NEM-RDFMG with DFs	1.13069	+3 pcm

Node Number	Difference in Relative Power (NEM-RDFMG – Serpent)	
	without DFs	with DFs
1	+0.06%	+0.00%
2	+0.06%	-0.01%
3	+0.07%	+0.00%
4	-0.35%	+0.00%
5	+0.07%	+0.00%
6	+0.07%	+0.01%
7	+0.07%	+0.01%

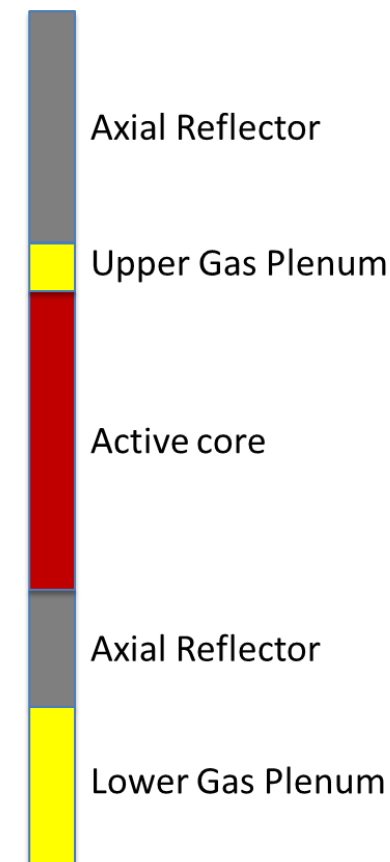
Based on AEN-WPRS SFR Core Definitions (v. 1.2)\*  
carbide core geometry and compositions.

### Axial DF Test

1 fuel assembly (30 axial nodes), radial  
reflective, axial vacuum boundary  
conditions

Code	Eigenvalue	Error
Serpent	1.02693	-
NEM-RDFMG without ZDFs	1.03190	+497 pcm
NEM-RDFMG with ZDFs	1.02710	+17 pcm

Node Number	Difference in Relative Power (NEM-RDFMG – Serpent)	
	Without ZDFs	With ZDFs
12	+0.65%	-0.05%
13	+0.06%	-0.02%
14	-0.06%	+0.02%
15	-0.14%	+0.06%
16	-0.21%	+0.07%
17	-0.23%	+0.07%
18	-0.20%	+0.04%
19	-0.18%	-0.02%
20	-0.09%	-0.06%
21	+0.40%	-0.10%



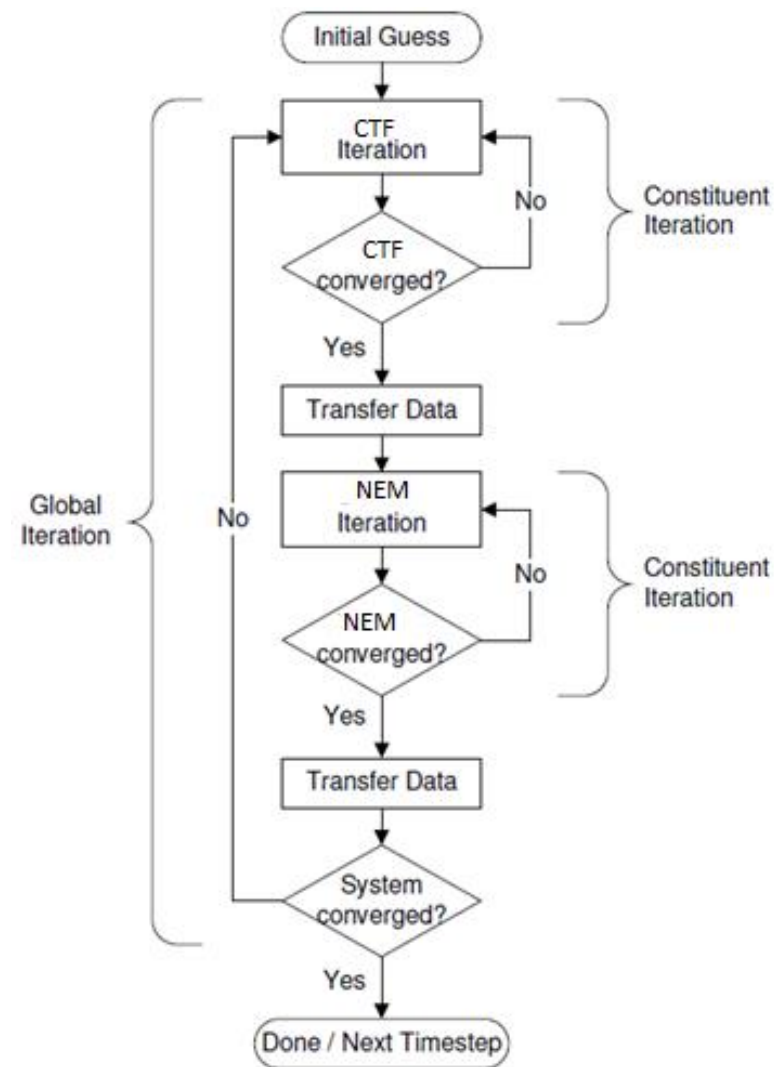
\*D. Blanchet, L. Buiron, N. Stauff, T. K. Kim and T. Taiwo, "AEN - WPRS Sodium Fast Reactor Core Definitions," Version 1.2.



## NEM/CTF/CTFFuel Coupling

An initial coupling has been utilizing Message Passing Interface (MPI) communication protocol to exchange thermal hydraulic data from CTF/CTFFuel to NEM and power profiles from NEM to CTF/CTFFuel.

- Coupling is external, temporally explicit.
- Coupling was developed specifically to include two T-H parameters (moderator density and fuel temperature).
- Hex-z geometry for SFRs has not yet been tested, however both codes have been demonstrated for SFRs and node to subchannel mapping is done in such a way that no geometry-related issues are anticipated.



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## Under-Development Thermal Expansion Solver

A basic expansion calculation capability is needed for both CTF/CTFFuel and NEM codes.

Due to the complexity of developing a complete thermo-mechanical code including interaction with structural components, pressures, etc., initial implementation considers:

- Simplified modelling through thermal expansion coefficients/linear expansion factors.
- Recalculation of subchannel/nodal geometries based on expansions.
- Basic geometry management to prevent unphysical configurations.

Even a simplified expansion calculation will promote the development of multi-physics interfaces in NEM/CTF/CTFFuel that will support continued thermo-mechanical solver development or integration.

Due to the close relation between the thermal hydraulics calculation and thermal expansion, the expansion solver is being implemented as a module directly interfaced with CTF in order to utilize and modify the CTF geometry on-line.



## Thermal Expansion Solver Interfaces

### CTF/CTFFuel:

- Expansion of fuel-internals: modification of fuel temperature calculation by manipulation of material properties and gap (sodium bond) conductance based on expansion – some existing capability through fuel deformation models, or direct modification of rod geometries.
- Expansion of cladding: modification of subchannel geometries.
- Expansion of diagrid: may be sufficient to evaluate ahead of time in most cases, or through modification of inter-assembly subchannels assuming inter-assembly flow is modelled.

### NEM:

- Modification of node size for diagrid expansion effects.
- Other expansions can be managed via cross section parameterization (radial expansions) together with a mixing method or parameterized axial discontinuity factors (axial expansions).

## Conclusions

- The subchannel code CTF has been extended to SFR-modelling and is undergoing further developments, verification and validation.
- Improvements of CTF wire-wrapped bundle modelling through Hi2Lo information from high-fidelity codes are planned in the near future.
- Development of improved CTFFuel gap conductance modelling underway.
- Initial work has been completed to incorporate CTF/CTFFuel in a coupled multi-physics scheme with the nodal neutronics code NEM, which has re-enabled hexagonal-z geometry capabilities and been integrated in a Hi2Lo scheme with the Monte Carlo code Serpent for cross section generation and equivalence (discontinuity factors).
- The multi-physics platform is being extended to include basic thermal expansion capabilities to support the development of thermal expansion interfaces and capabilities for CTF/CTFFuel and NEM.

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