# MULTISCALE COMPUTER SIMULATION OF FISSION GAS DISCHARGE DURING LOSS-OF-FLOW ACCIDENT IN SODIUM FAST REACTOR

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## **Abstract**

The required technological and safety standards for future Gen IV Reactors can only be achieved if advanced simulation capabilities become available, which combine high performance computing with the necessary level of modeling detail and high accuracy of predictions. The development of a suite of high performance computational tools for multiscale simulations of Gen-IV Sodium Fast Reactor (SFR) has been undertaken by a DOE-sponsored university consortium (RPI, Columbia University and SUNY at Stony Brook).

## 1. INTRODUCTION

The purpose of this paper is to present a multiscale modeling approach for mechanistic three-dimensional transient computer simulations of the injection of a jet of gaseous fission products into a partially blocked SFR coolant channel following localized cladding overheat and breach. Schematics of the proposed SFR and of the consequences of local cladding failure are shown in Figs. 1 and 2. The phenomena governing accident progression have been resolved at three different spatial and temporal scales by the inter-communicating computational multiphase fluid dynamics (CMFD) codes: FronTier, PHASTA and NPHASE-CMFD. A brief description of the major features of the individual codes is given in the Section 2 below.

The smallest (mm) scale phenomena under consideration deal with the failure of an overheated fuel rod cladding and the subsequent fission gas discharge through the cladding breach into the liquid sodium coolant. The underlying processes are resolved using the FronTier code.

The intermediate (cm range) scale of the simulation deals with the fission-gas-jet formation along a short section of the coolant channel around the cladding breach region. Using the geometry of the breach and the gas injection flow rate calculated by FronTier, a combined DNS/Level-Set simulation of two-phase turbulent flow is performed by the PHASTA code. The turbulent two-phase PHASTA outflow is then averaged over time to obtain mean phasic velocities and volumetric concentrations, as well as the liquid turbulent kinetic energy and turbulence dissipation rate, all of which serve as the input to the next (macro) scale of simulations. A sliding window time-averaging has been used to capture the mean flow parameters for transient cases.

The largest scale (m range) of the simulation considers the flow of liquid sodium-coolant/fission-gas mixture along the length of fuel elements. This simulation has been performed by NPHASE-CMFD code using the RANS modeling scale. NPHASE-CMFD uses two-phase k- $\epsilon$  models along with transient inflow boundary conditions supplied by PHASTA to perform two- (or multi) phase flow simulations during the postulated accident. NPHASE-CMFD also supplies the pressure value back to the PHASTA domain outflow. PHASTA, in turn, provides the pressure found at the inflow of its domain back to the FronTier outflow. Thus, all three codes used in the simulations are fully coupled. The use of such a multiple code platform allows one to perform full-scale mechanistic simulations of hypothetical reactor accidents, including both current and next generation reactors, while maintaining the required level of detail assured by the multiscale approach.

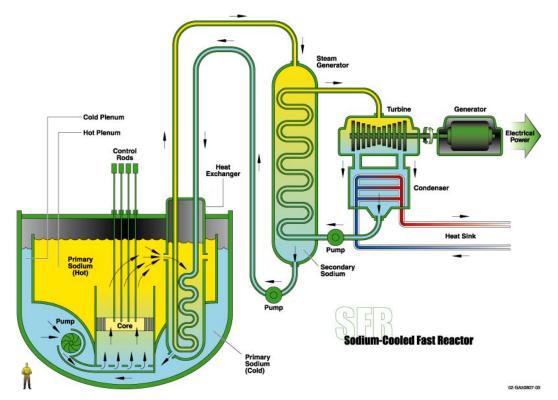


Fig. 1: A general schematic of a Gen-IV Sodium-Cooled Fast Reactor (Source: A Technology Roadmap for Generation IV Nuclear Energy Systems by the U.S. DOE Nuclear Energy Research Advisory Committee and the Generation IV International Forum)

## 2. DESCRIPTION OF INDIVIDUAL COMPUTER CODES

## 2.1. FronTier

FronTier is a computational package for direct numerical simulation of multiphase flows (Du et al., 2006) developed at Stony Brook University in collaboration with LANL and BNL. FronTier development and optimization for massively parallel supercomputers is a part of the DOE SciDAC program. An important and unique feature of this package is its robust ability to track dynamically moving fronts or material interfaces using the method of front tracking. FronTier supports compressible and incompressible Navier-Stokes equations and MHD equations in the low magnetic Reynolds number approximation (Samulyak, 2007), and phase transitions such as melting and vaporization (Wang et al., 2010).

## 2.2. PHASTA

PHASTA (Whiting and Jansen, 2001; Jansen et al., 2000) is a parallel, hierarchic (between 2nd-and 5th orders of accuracy, depending on function choice), adaptive, stabilized (finite element) transient analysis DNS flow solver (both incompressible and compressible). PHASTA was the first unstructured grid LES code, and it has been applied to turbulent flows ranging from validation benchmarks (channel flow, decay of isotropic turbulence) to complex flows (airfoils at maximum lift, flow over a cavity, near lip jet engine flows and fin-tube heat exchangers). The PHASTA code uses advanced anisotropic adaptive algorithms (Sahni et al., 2006) and the most advanced LES/DES models (Tejada-Martinez and Jansen, 2005). The two-phase version of PHASTA utilizes the Level Set method to define the interface between the gas and liquid phases (Sethian, 1999). The combined DNS/Level-Set model has been extensively tested and validated for various two-phase flow problems and condiitons (Nagrath et al., 2005; Rodrigez, 2009).

# 2.3. NPHASE-CMFD

NPHASE-CMFD (Antal et al., 2000) is an advanced Computational Multiphase Fluid Dynamics computer code for the simulation and prediction of combined mass, momentum and energy transfer processes in a variety of single-phase (Gallaway et al., 2008) and multiphase/multiscale systems, including gas/liquid (Wierzbicki et al., 2007; Tselishcheva et al., 2010), solid/liquid (Tiwari et al., 2006; 2009) and gas/solid/liquid (Antal et al., 2000) flows. It uses two-phase k-ε models of turbulence (the user can chose between the High Reynolds Number and Low Reynolds Number options of the model). The mixture and field continuity equations are solved in coupled and segregated (uncoupled) manner, using stationary coefficient linearization. The code is fully unstructured and can utilize second-order accurate convection and diffusion discretization. The technology used by the NPHASE-CMFD code is an ensemble averaged multifield model of two-phase or multiphase flows.

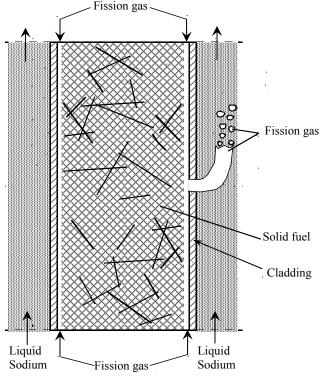


Fig. 2. Schematic of fission gas escape in SFR during fuel rod failure accidents.

## 3. MODEL DESCRIPTION

## 3.1. Physical Problem

As it was mentioned before, a hypothetical channel-blockage accident scenario in Gen-IV SFR has been used as testing ground for the proposed approach of using three interacting codes in multiscale simulations. Fig. 3 presents an overview of the problem geometry. It has been assumed that as a result of the accident, one of the fuel rods overheats and causes a failure of the stainless steel cladding. This results in fission gas injection into the coolant.

The modeled phenomena include:

- stainless steel failure mechanisms
- pressurized fission gas escape from the fuel rod into the liquid sodium coolant
- two-phase side jet injection into the coolant
- transient two-phase flow propagation downstream from cladding failure

## 3.2. Computational Domains

Figure 4 shows the computational domain sharing in the multiscale approach used in the simulations. Let us overview the main reasons for choosing the multiscale approach consisting of the three different scales:

- The largest scale simulation performed using NPHASE-CMFD code is capable of resolving the whole fuel rod assembly. However, to achieve that we employ RaNS equations with quite coarse mesh resolution (about 5 to 10 mesh cells between the fuel rods). This does not allow adequate model performance around the cladding failure.
- DNS approach is used within 10 mm of cladding failure using PHASTA code. The unstructured mesh capabilities of PHASTA allow modeling the jet propagation in the complex flow domain between the fuel rods.
- FronTier is resolving the fission gas flow though the growing crack in the stainless steel cladding in the immediate vicinity of the failure.

A description of the domain used by each of the three codes and their interfaces is given next.

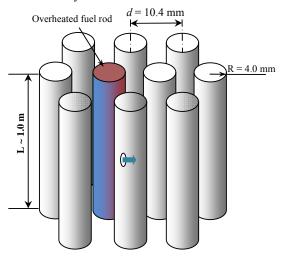


Fig. 3. Geometry and dimensions of a section of SFR fuel rod assembly with the cladding failure location.

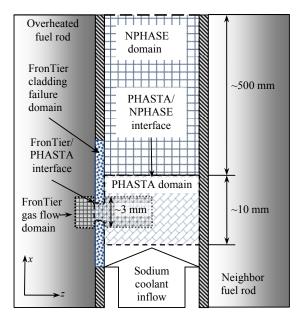


Fig. 4. Computational domains overview.

# 3.2.1. FronTier computational domains

FronTier simulates both cladding failure and fission gas escape through the failure. The cladding failure computational domain includes a short section of the cladding tube. The fluid flow domain includes small regions about 3 mm in size inside and outside the stainless steel cladding and resolves the gas jet using a rectangular grid. Since FronTier must use uniform grid it is suitable to relatively small domains and restricted to the region very close to the cladding breach. Computational grid used in the FronTier simulations of cladding breach is shown in Fig. 5 (a).

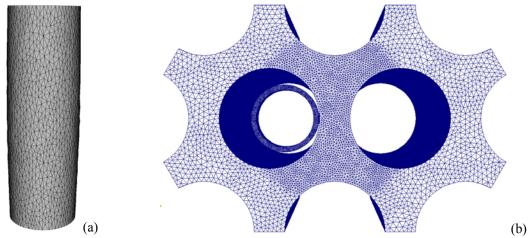


Fig. 5. Computational meshes used in the FronTier simulations of cladding breach (a) and PHASTA simulations (b).

## 3.2.2. PHASTA computational domain

The PHASTA domain is about 10 mm tall and includes the region around the cladding breach, which overlaps with the FronTier domain, as well as section of the coolant channel which starts below the breach and extends to a short distance above the breach. The finite element mesh used in PHASTA simulation is shown in Fig. 5 (b). It is characterized by the following parameters:

- Number of vertices: 1.52 million
- Number of elements: 8.36 million

The computational mesh has been designed to provide adequate resolution for interface tracking in the region of interest. This mesh accurately captures the near-wall (inside the boundary layer) flow details for both laminar and turbulent flow conditions. As an illustration, Fig. 6 shows that the PHASTA predictions are in excellent agreement with the fundamental "law of the wall" for turbulent flows.

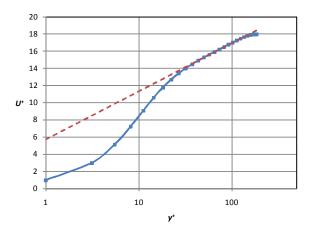


Fig. 6. PHASTA velocity profile in turbulent channel flow compared with law of the wall (Bolotnov et al., 2009).

The gas flow rate computed by FronTier simulations is used for setting up gas inflow boundary conditions in PHASTA. Other boundary conditions are: no-slip boundary conditions applied on all solid surfaces, and a pressure boundary condition that corrects for the effects of surface tension at the outflow of the domain. This outflow pressure is supplied by the NPHASE flow solver.

## 3.2.3. NPHASE computational domain

The computational domain of NPHASE, shown in Fig. 4, actually encompasses and extends along the coolant channels around 30 fuel rods. This is shown in Fig. 7 (a), where the NPHASE domain overlays the PHASTA domain. Due to the symmetry of the problem and the ensemble averaged nature of the NPHASE calculation, the data taken from PHASTA is averaged across the symmetry line shown in Fig. 7 (a). The corresponding computational mesh in the NPHASE simulations is shown in Fig. 7 (b).

The mesh used in the NPHASE simulation is shown in Fig. 7 (b). It is axially non-uniform and consists of approximately 500k elements. Since the NPHASE mesh is much coarser than the PHASTA mesh, data is interpolated from the PHASTA onto the NPHASE meshes to generate the inlet conditions for the NPHASE simulation. The total physical length of the NPHASE domain is 0.5m. This, in turn, illustrates the advantages of coupling the DNS results of PHASTA, limited for practical reasons to a relatively small computational domain, with the NPHASE-based large-scale model which uses accurate PHASTA predictions as input (Bolotnov et al., 2009).

# 3.3. Description of mathematical models

#### 3.3.1. FronTier Models

The FronTier package has the ability to evaluate moving fronts or material interfaces using the method of front tracking. A volume-filling finite difference grid supports smooth solutions located in the region between interfaces. In the FronTier's solution algorithm (Menikoff and Plohr, 1989), the Riemann problem is solved for the left and right interface states to predict the location and states of the interface at the next time step. Then a corrector technique is employed which accounts for fluid gradients on both sides of the interface.

For the simulation of overheating and melting of the nuclear fuel rod, new elliptic/parabolic solvers have been developed, based on the embedded boundary method (Wang et al., 2010), as well as an algorithm for the classical Stefan problem describing first order phase transitions.

A new approach, based on the energy minimization of the network of springs with critical tension, has also been applied to develop mesoscale models for the simulation of fracture of inhomogeneous solid materials. Such a description of solids makes it possible to avoid fast time scales associated with acoustic waves and capture important features of the material fracture. The main emphasis has been on the study of brittle fracture. Two regimes of the fracture have been considered: (a) adiabatically slow deformation and breakup and (b) instantaneously fast deformation and the formation and propagation of cracks in stressed materials. The most computationally intensive step in the algorithm is the energy minimization. The methodology applied to both constrained and unconstrained optimization problems is done through the interface with TAO, a package developed by Argonne National Lab within the DOE SciDAC initiative.

Model testing included a comparison of the breakdown stress with experimental data, studies of the breakdown stress as a function of the probability of defects up to the rigidity percolation threshold, and scaling of the distribution function of the breakdown stress.

## 3.3.2. PHASTA models

The spatial and temporal discretization of the Incompressible Navier-Stokes equations within PHASTA has been described in Whiting and Jansen (2001). The strong form of the INS equations is given by

Mass conservation 
$$u_{i,j} = 0$$
 (1)

Momentum conservation 
$$\rho u_{i,t} + \rho u_{j} u_{i,j} = -\hat{p}_{,i} + \hat{\tau}_{ii,j} + \hat{f}_{i}$$
 (2)

where  $\rho$  is density,  $u_i$  is the *i*-th component of velocity,  $\hat{p}_{,i}$  is pressure,  $\hat{\tau}_{ij}$  is the stress tensor, and  $\hat{f}_i$  represents body forces along the *i*-th coordinate.

For the incompressible flow of a Newtonian fluid, the stress tensor is related to the strain rate tensor,  $S_{ij}$ , as

$$\hat{\tau}_{ii} = 2\mu S_{ii} = \mu(u_{i,i} + u_{i,i}) \tag{3}$$

Using the Continuum Surface Tension (CST) model of Brackbill et al. (1992), the surface tension force is computed as a local interfacial force density, which is included in  $\hat{f}_i$ .

The stabilized finite element formulation is used in the PHASTA code (Whiting and Jansen, 2001). The level set method (Sethian, 1999) involves modeling the interface as the zero level set of a smooth function,  $\varphi$ , where  $\varphi$  represents the signed distance from the interface.

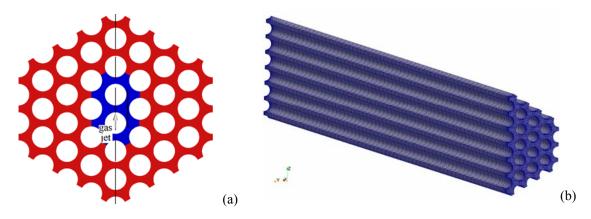


Fig. 7. NPHASE-CMFD domain: (a) Cross section of the NPHASE domain showing overlap with the PHASTA domain (blue) and the added coolant channels (red), the arrow indicates the location of gas jet injection. (b) Computational mesh used in the NPHASE simulations.

## 3.3.3. NPHASE physical model

The multiphase model in the NPHASE-CMFD code is based on the multifield modeling concept. The ensemble-averaged mass and momentum equations, respectively, are given by

Mass conservation 
$$\frac{\partial (\alpha_k \rho_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \overline{\mathbf{v}}_k) = \Gamma_k \tag{4}$$

Momentum conservation 
$$\frac{\partial \left(\alpha_{k}\rho_{k}\overline{\mathbf{v}}_{k}\right)}{\partial t} + \nabla \cdot \left(\alpha_{k}\rho_{k}\overline{\mathbf{v}}_{k}\overline{\mathbf{v}}_{k}\right) = -\alpha_{k}\nabla \overline{p}_{k} - \sum_{j}(\overline{p}_{k} - p_{kj}^{i})\nabla \alpha_{k} \\ + \alpha_{k}\nabla \cdot \underline{\overline{\mathbf{t}}}_{k}^{i} + \sum_{j}(\underline{\overline{\mathbf{t}}}_{k}^{i} - \underline{\mathbf{t}}_{kj}^{i})\nabla \alpha_{k} + \sum_{j}\mathbf{M}_{kj}^{i} + \alpha_{k}\rho_{k}\mathbf{g}$$

$$(5)$$

In Eqs.(4)–(5), (j,k) are the field indices, the subscript 'i' refers to the interfacial parameters,  $\mathbf{M}_{kj}^{i}$  is the interfacial force per unit volume exerted by field-j on field-k, and the remaining notation is conventional.

# 3.4. Boundary conditions and interfaces between the codes

To achieve coupling between the three codes used in the analysis, a consistent data transfer must be provided between the individual codes. A file-based data transfer method has been used to transfer the multiphase inflow boundary conditions needed by the "downstream" software using additional processing, such as space and time interpolation as well as averaging techniques when converting the DNS results into RaNS inflow boundary conditions. In order to fully couple the codes, a pressure feedback has been developed as a data transfer method from NPHASE-CMFD to PHASTA and from PHASTA to FronTier. Once this feedback is fully implemented, the PHASTA and FronTier time-transient solutions will directly depend upon the large scale dynamics modeled by NPHASE-CMFD.

## 3.4.1. FronTier to PHASTA interface description

The FronTier crack formation simulation generates mesh coordinates along with a connectivity array for the crack shape at each time step of the crack growth simulation. The PHASTA simulation uses this information to block selected internal mesh nodes in its computational domain, to dynamically change the effective crack size in the two-phase flow simulation.

Since both FronTier and PHASTA provide instantaneous velocity fields as their solutions, no averaging of the data is required for this interface. The following steps are taken to use the fission gas velocity profile flowing though the failed stainless steel cladding opening computed by FronTier as PHASTA inflow boundary conditions:

- Velocity distribution is recorded by FronTier in the plane of interest
- For each FronTier time step velocity profiles are interpolated on the PHASTA mesh inflow nodes
- During the PHASTA run the time-dependent velocity profiles from FronTier are used as jet inflow boundary conditions (linear time interpolation is performed when PHASTA time step is smaller than FronTier time step)

#### 3.4.2. PHASTA to NPHASE-CMFD data transfer

The DNS results produced by the PHASTA code require averaging before they can be used in NPHASE-CMFD as inflow boundary conditions. The following technique is used to provide the boundary conditions for the NPHASE domain:

- A list of coordinates at the NPHASE domain inflow is generated.
- At every time step of PHASTA execution instantaneous velocity components  $(u_1, u_2, u_3)$  and distance to interface field are interpolated from PHASTA solution at the NPHASE coordinates.
- A postprocessing code performs the analysis of the data and computes the mean velocity distribution  $(U_1^k, U_2^k, U_3^k)$ , volume fraction, turbulent kinetic energy and turbulence dissipation rate, for each flow field, k (e.g., k = 1 for liquid and k = 2 for gas).

For transient flow we perform sliding window averaging. The analysis results in the following time-dependent functions of the described quantities:

$$U_{i}^{k}(t) = \frac{1}{\alpha_{k} N_{w}} \sum_{i=1}^{N_{w}} X_{k} u_{m}^{i} \left(t + t_{j}\right) \qquad k^{k}(t) = \frac{1}{\alpha_{k} N_{w}} \sum_{i=1}^{N_{w}} X_{k} \sum_{i=1}^{3} \frac{1}{2} \left(u_{m}^{\prime i} (t + t_{j})\right)^{2}$$
 (6)

$$U_{i}^{k}(t) = \frac{1}{\alpha_{k} N_{w}} \sum_{j=1}^{N_{w}} X_{k} u_{m}^{i} \left(t + t_{j}\right) \qquad k^{k}(t) = \frac{1}{\alpha_{k} N_{w}} \sum_{j=1}^{N_{w}} X_{k} \sum_{i=1}^{3} \frac{1}{2} \left(u_{m}^{ii}(t + t_{j})\right)^{2}$$

$$\varepsilon^{k}(t) = v \frac{1}{\alpha_{k} N_{w}} \sum_{j=1}^{N_{w}} \sum_{i=1}^{3} \sum_{k=1}^{3} X_{k} \frac{\partial u_{m}^{ii}(t + t_{j})}{\partial x_{k}} \qquad \alpha_{k}(t) = \frac{1}{N_{w}} \sum_{j=1}^{N_{w}} X_{k}(t + t_{j})$$

$$(6)$$

where  $X_k$  is the phase indicator function for field k,  $u_m^{i}(t+t_j) = u_m^i(t+t_j) - U_i(t)$  is the fluctuation of velocity component i computed during the ensemble run m at the time instant  $t + t_i$ ;  $N_w$  is the number of velocity samples in each window, t is the current time,  $t_i = (j - N_w/2)\Delta t$  is the local window time,  $\Delta t$  is the time step.

## 4. RESULTS

The models discussed in Section 3 have been used to simulate the consequences of a loss-of-flow accident in a Gen. IV Sodium fast reactor (SFR). The phenomena modeled included: fuel element heatup, cladding heatup and failure due to combined effects of thermal stresses and fission gas pressure inside the fuel pin, injection of pressurized fission gas into the coolant channels surrounding the failed fuel element, and the transport of gas/liquid-sodium mixture toward the top of the core. The results of the multiscale simulations are presented next.

## 4.1. FronTier Calculations

The cladding fails before melting, causing the ejection of fission gases into the coolant channels. The increasing fuel temperature causes the pressure inside the fuel rod to increase as well, thus augmenting the mechanical load on the cladding wall. The combined effects of elevated gas pressure and cladding temperature weaken the cladding wall and eventually lead crack formation. The predicted crack side is shown in Fig. 8. The FronTier code was used for the simulation of the fission gas ejection into the sodium coolant. Boundary conditions behind the crack were estimated based on the flow in porous medium equations describing the flow of fission gases from the gas plenum to the crack. The gas jet simulation (see Fig. 9) provided input to the PHASTA code.

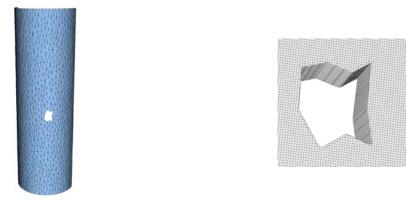


Fig. 8. Formation of crack in the fuel rod cladding (left). Magnified view of the crack surface with mesh for the FronTier simulation of the gas jet ejection is shown on the right.

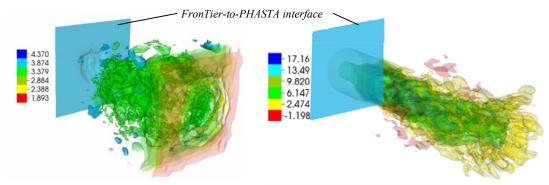
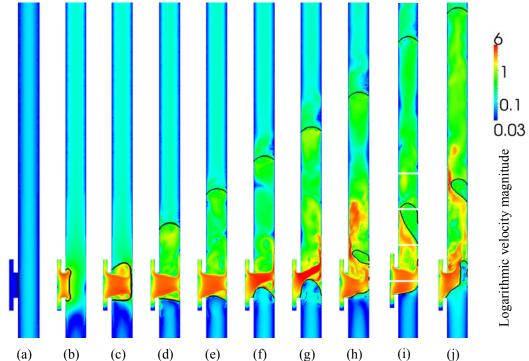


Fig. 9. Fron Tier simulation of the ejection of fission gas into sodium coolant: isosurfaces of pressure (left) and longitudinal component of velocity (right) at 1 ms after the crack formation.

## 4.2. PHASTA Calculations

The PHASTA code has been used to perform the two-phase DNS of the jet injection. Once the codes are fully coupled, it will use the gas inlet information provided by FronTier (Fig. 9) to simulate a time-varying crack shape with time-dependent gas inflow profile. A set of numerical test has been performed to develop and test PHASTA ability to handle variable gas inflow profiles through growing crack shapes. These numerical tests have shown that PHASTA is capable in accepting the FronTier information about the arbitrary crack shape and gas velocity profile. Current results use simplified assumptions about the crack shape (a rectangular shape 3 mm long and 1 mm wide) and a constant gas flow rate. Side cuts of the instantaneous PHASTA solution development are shown in Fig. 10. We can observe how the fission gas jet behaves during the modeled accident scenario. Note that the simulation time is quite short for the conditions under consideration (liquid volume flow rate is  $18.2 \times 10^{-6}$  m³/s; gas volume flow rate is  $10.1 \times 10^{-6}$  m³/s in the domain enclosing 2 fuel rods).

In order to better illustrate the behavior of the gas jet simulation we chose time instant of 0.18 s to provide several domain cuts normal to the coolant flow direction (Fig. 11). The locations of these cuts are shown as white lines in Fig. 10 (i). The present two-phase PHASTA simulation was performed on 2,048 IBM BlueGene/L processors for about 250 wall clock hours, which corresponds to approximately 500,000 CPU-hours. The PHASTA simulation results are averaged using a plane of virtual probes located normal to the coolant flow direction at the distance of 7 mm from the center of the fission gas inflow. The location of the data gathering plane is shown by a white gap between the computational domains in Fig. 12. The averaged data is then supplied to the NPHASE-CMFD RANS based simulation of as the inflow boundary conditions.



(a) (b) (c) (d) (e) (f) (g) (h) (i) (j) Fig. 10. Time evolution of the instantaneous PHASTA velocity field. The gas/liquid interface is marked with a solid black line. Each instant corresponds to the following computational time: (a) 0.0 s; (b) 0.0003 s; (c) 0.003 s; (d) 0.03 s; (e) 0.06 s; (f) 0.09 s; (g) 0.12 s; (h) 0.15 s; (i) 0.18 s; (j) 0.21 s.

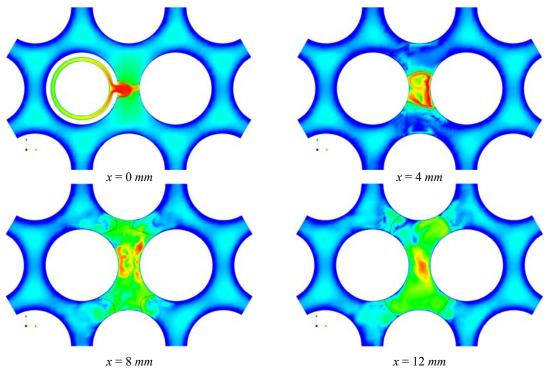


Fig. 11. Two-phase velocity distribution around the fuel rods at different locations downstream of the center of the gas jet. The time instant is 0.18 s and velocity scale is the same as in Fig. 10.

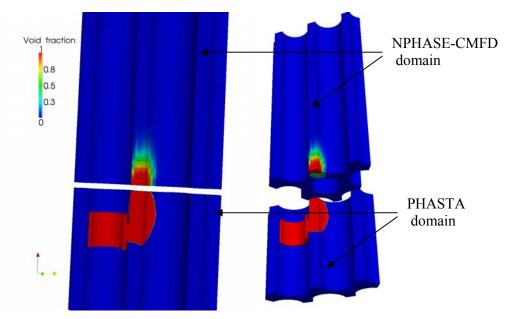
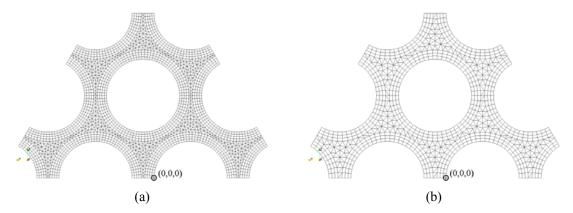


Fig. 12. PHASTA/NPHASE-CMFD data transfer: PHASTA domain (bottom part) computes gas (red) / liquid (blue) phase distributions which are averaged to provide the time-varying inflow to NPHASE domain (volume fraction distribution shown on top).

## 4.3. NPHASE-CMFD Calculations

The NPHASE-CMFD code has been used to simulate the largest scale part of the present multiscale problem. To study the accuracy of NPHASE-CMFD results, a grid-convergence study has been performed for a complex geometry of reactor fuel channels. Two grids have been compared against each other: a coarse grid of about 45K elements, shown in Fig. 13(a), and a fine grid of about 180k elements, shown in Fig. 13(b).



**Fig. 13**: Cross sectional views of two computational grids used in this study of grid-independence of NPHASE-CMFD calculations, (a) fine grid, (b) coarse grid.

These two grids were run for a steady state simulation closely matching the expected conditions of the PHASTA/NPHASE coupled gas jet. The case examined in the grid study uses an assigned gas distribution at the inlet as well as constant velocity values for both the liquid and gas phases. The calculated axial velocity components of both gas and liquid phases, as well as the gas volume fraction, along the main flow direction are shown in Fig. 14. As it can be seen, the results for the coarse grid are very close to those for the fine grid. Similar conclusions can be drawn from Fig. 15, where the lateral profiles are shown of both the axial phasic velocities and gas volume fraction. Thus, one concludes that the "coarse" mesh yields accurate, practically grid-independent results.

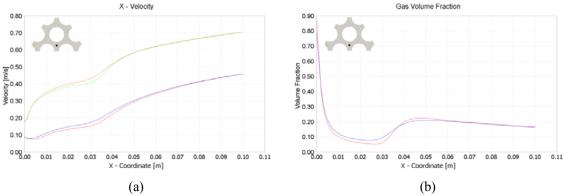


Fig. 14: Axial distributions of the: (a) x-velocity components of both liquid and gas phases, and, (b) volume fraction of the gas phase for the fine and coarse grids. The red and green lines represent the fine grid whereas the blue and orange lines represent the coarse grid.

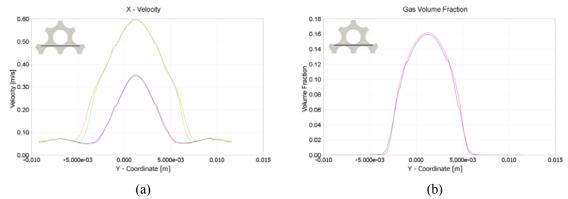


Fig. 15: Lateral (i.e., across the y axis) distributions at x = 0.09 cm of the: (a) x velocity components of both phases and (b) volume fraction of the liquid and gas phases for the fine and coarse grids. The red and green lines represent the fine grid whereas the blue and orange lines represent the coarse grid.

The data has been collected at a cross plane in the PHASTA domain and used at the inlet of the NPHASE simulation. The inflow data taken from the PHASTA simulation has been applied to the blue region shown in Fig. 7 (a). For the inlet condition used in the NPHASE domain in the regions not covered by the PHASTA simulation, a fully developed turbulent profile has been used matching the coolant mass flux specified by PHASTA. This profile has been calculated using the NPHASE code.

The NPHASE-CMFD model has been used to determine how the gas released into the coolant spreads as it travels along the coolant channel. Fig. 16 (c) shows how the volume fraction of gas changes along the reactor channel. The turbulent dispersion force causes it to spread out over a significant portion of the channel cross section. The NPHASE model tracks the velocity fields of the gas and liquid phases independently. These can be seen in Figs. 16 (a) and 16 (b). The complex inlet flow pattern is a direct result of large scale eddies produced by the jet hitting the neighboring fuel rods. These are long standing fluid structures which are not eliminated by the time averaging done on the PHASTA data. Downstream from the jet, these structures decay into a much less chaotic flow. As can be seen in Fig. 16 (b), the gas velocity increases along the channel due to gravity. This causes a drop in volume fraction which is observed in the initial section of the channel.

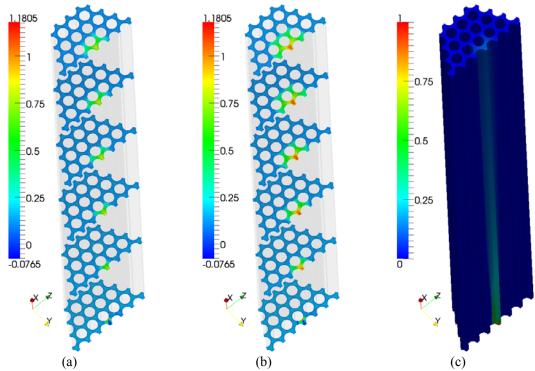


Fig. 16. (a) U velocity component of liquid phase; (b) U velocity component of gas phase; (c) volume fraction of the gas phase in the NPHASE solution (inlet at bottom, outlet at top, equally-spaced intervals in between).

## 5. SUMMARY AND CONCLUSIONS

A multiscale modeling approach to the analysis of nuclear reactor transients and accidents has been discussed. It has been demonstrated that by using multiple computer codes in a coupled mode (NPHASE/PHASTA interface), a broad range of phenomena governing accident progression can be simulated in a physically-consistent and numerically accurate manner. Future work will include the development of a closer coupling between FronTier and PHASTA, and the modeling of multicomponent flows, such as molten/frozen fuel particles mixed with fission gas, and the effect of sodium bubbles mixed with the evaporating liquid sodium.

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