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Reactor Core Sub-Assembly Simulations Using a Stabilized Finite Element Method

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Abstract

This paper presents a methodology for solving thermal-hydraulic flows that are prototypical to nuclear reactors, based upon a stabilized finite element method. The flow equations including both steady-state and transient turbulence models and conjugate heat transfer are solved with a fully-coupled algebraic multigrid (AMG) preconditioned Newton-Krylov iterative solver. Of special interest is the efficiency and weak scaling behavior of the AMG based preconditioners, tailored for steady-state solves and those tailored for short time-scale transient time marching, as the problem size increases. These studies will be useful in predicting computational resource requirements necessary to perform full-scale single- and multi-physics simulations. These studies will also provide a baseline performance level for future turbulence model and solver development.

Introduction

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is the name of a new U.S. Department of Energy Innovation Hub that is investing in the development of a "virtual reactor toolkit" that incorporates science-base models, state-of-the-art numerical methods, modern computational science and software engineering, uncertainty quantification (UQ) and validation against currently operating pressurized water reactors. Under CASL there are five focus areas with different responsibilities. One of these, Modeling and Numerical Methods (MNM) is tasked with developing computational fluid dynamics (CFD), multi-phase computational fluid dynamics (MCFD) and thermal-hydraulics (TH) codes that can simulate challenge problem flows.

One of the challenge problems deals with grid-to-rod-fretting (GTRF). This problem is characterized by flow induced rod vibrations that cause deterioration of the rod cladding material and support grids at points of contact. The vibrations are due to turbulent flow generated at the core inlet and by rod bundle support grid mixing vanes. Turbulence is deliberately generated to enhance heat transfer and prevent localized hot spots from occurring. This problem is inherently three-dimensional and unsteady. Better understanding of excitation phenomena through high-

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fidelity simulations has the potential to improve clad time-to-failure, and improve reactor core performance.

Ultimately, full-scale simulations of the entire reactor core including inlet/outlet characterization will be performed. Included in these will be coupled fluid/structure interaction simulations. Leading up to full-scale, various sub-scale rod bundle assemblies serving as prototypes will be simulated and analyzed. Separate fluid and structural dynamic simulations will be conducted where the rod excitation predicted by the fluid simulations will be transfered to the structural code through surface boundary conditions.

Our initial prototype problem is a turbulent simulation of a 3x3 rod bundle with support grid. Both unsteady Reynolds averaged Navier-Stokes (URANS) and large-eddy simulation (LES) turbulence model methodologies will be employed. Several models will be evaluated based on solution data. Also, of particular interest is how well recently developed linear system solver preconditioners perform on these high Reynolds number transient flows.
This work follows closely the work by Benhamadouche et al.[1] who used an unstructured finite-volume discretization and SIMPLEC iteration procedure to solve the flow equations.

1. Governing equations

This section describes the governing equations for modeling turbulent single-phase flows that are currently under development in the TH code. The code is currently designed to solve the low-flow Mach number Navier-Stokes system with coupled heat transfer, and chemical species transport with non-equilibrium bulk and surface phase reactions. The code also has the capability to include heterogeneous multiphysics formulations such as fluid flow and conjugate heat transfer and/or chemically reacting transport.

1.1 Flow equations

A summary of the governing equations is presented in Table 1.

Governing Equation	
Continuity	$R_\rho = \frac{\partial \bar{\rho}}{\partial t} + \bar{\rho}\nabla \cdot \tilde{\mathbf{u}}$
Momentum	$R_m = \frac{\partial(\bar{\rho}\tilde{\mathbf{u}})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}}) + \nabla \cdot \mathbf{T} - \bar{\rho}\mathbf{f}_i$
Energy	$R_T = \frac{\partial(\bar{\rho}C_p\tilde{T})}{\partial t} + \nabla\cdot(\bar{\rho}C_p\tilde{T}\tilde{\mathbf{u}}) + \nabla \cdot \mathbf{q} + \nabla \cdot \mathbf{q}_r - \nabla \cdot \phi$

Table 1. Summary of governing equations.

In these equations, $\bar{\rho}$ is the density, $\tilde{\mathbf{u}}$ is the velocity vector, and C_p is the specific heat. Also, $\mathbf{T}$ represents the stress tensor (containing pressure, P)

$$\mathbf{T} = P\mathbf{I} + \mu_{eff}\left[\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^T\right] - \frac{2}{3}\mu_{eff}\left(\nabla\cdot\bar{\mathbf{u}}\right)\mathbf{I},$$

I is identity matrix, **q**, the heat flux vector,

$$\mathbf{q} = -\lambda_{eff}\nabla\bar{T}$$

and $\mathbf{q}_r$, the heat flux vector due to radiation. The "eff" subscript on viscosity and conductivity signifies that these coefficients contain both molecular and eddy viscosities,

$$\mu_{eff} = \mu + \mu_t, \quad \lambda_{eff} = \lambda + \lambda_t, \quad \lambda_t = \frac{\mu_t C_p}{\mathrm{Pr}_t}.$$

The bar/tilde denotes time/ensemble averaging in the context of URANS and spatial filtering in LES. The filter operator is mass weighted (Favre) if density is not constant. The turbulent Prandtl number Pr_t, is user specified. Note that the dissipation

$$\phi = \left(\bar{\boldsymbol{\tau}}\cdot\nabla\right)\bar{\mathbf{u}}$$

can be neglected in certain situations because in general the kinetic energy is much less than the internal energy. This assumption will be evaluated on a case-by-case basis.
It should be noted that there are several versions of the energy equation that could be substituted for the temperature equation listed in Table 1. The code can accommodate any of these and the most appropriate one will be chosen on a case-by-case basis. Boundary conditions common to most fluid dynamics codes will be required. Among these are inflow/outflow, no-slip surface and periodic.

1.2 Turbulence equations

The Reynolds number for this class of flows can typically reach tens of thousands and sub-assembly hardware can be several meters in length rendering direct numerical simulation un-tractable. It is therefore necessary to apply averaging or filtering to the governing equations resulting in URANS and LES models for turbulent flows. This section presents the model equations and several specific models that are evaluated for the rod bundle sub-assembly flow problem.

1.2.1 Reynolds Averaged Navier-Stokes

The effect of turbulence is modeled using the Boussinesq approximation relating Reynolds stress to the resolved strain rate;

$$\tau_t = -\bar{\rho}\widetilde{\mathbf{u}''\mathbf{u}''} = \mu_t\left[\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^T\right] - \frac{2}{3}\left[\mu_t\left(\nabla\cdot\bar{\mathbf{u}}\right) + \bar{\rho}k\right]\mathbf{I}$$

and is coupled to the momentum and energy equations through the eddy-viscosity. Here *k* is the turbulent kinetic energy that appears in some RANS models such as the $k-\varepsilon$ model.

1.2.1.1 Spalart-Allmaras model

The Spalart-Allmaras one-equation eddy viscosity model [2] will be utilized due to it's simplicity and robustness. While not widely used by the thermal hydraulics modeling community, it is quite effective in situations of attached flows. The affects of turbulence are coupled to the Navier-Stokes equations through the eddy viscosity and turbulent heat flux. The transport equation is;

$$R_{SA} = \bar{\rho}\frac{\partial \hat{\upsilon}}{\partial t} + \bar{\rho}\vec{u}\cdot\nabla\hat{\upsilon} - \nabla\cdot\mu_{eff}\nabla\hat{\upsilon} + C_{w1}f_w\bar{\rho}\left(\frac{\hat{\upsilon}}{d}\right)^2 - C_{b1}\bar{\rho}\hat{\upsilon}\hat{S} - \frac{C_{b2}\bar{\rho}}{\sigma}\left(\nabla\hat{\upsilon}\right)^2$$

Table 2. Spalart-Allmaras RANS turbulence model.

The eddy viscosity is defined as; $\mu_t = \bar{\rho}\hat{\upsilon}f_{v1}$.

At no-slip surfaces the eddy-viscosity is zero and so the dependent variable in the Spalart-Allmaras equation is set to zero there.

1.2.1.2 $k-\acute{U}$ model

Additional RANS models that will be investigated are derived from a family of two equation eddy-viscosity models that include the turbulent kinetic energy equation along with an equation that describes the local turbulent scale determining equation such as the turbulent dissipation (presented here) or specific dissipation [3,4].

Turbulent Kinetic Energy	$R_k = \bar{\rho}\frac{\partial k}{\partial t} + \bar{\rho}\vec{u}\cdot\nabla k - \nabla\cdot\left(\mu + \frac{\mu_t}{\sigma_k}\right)\nabla k - P_k + \rho\varepsilon$
Turbulent Dissipation	$R_\varepsilon = \bar{\rho}\frac{\partial \varepsilon}{\partial t} + \bar{\rho}\vec{u}\cdot\nabla\varepsilon - \nabla\cdot\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon - f_1 C_{\varepsilon 1}\frac{\varepsilon}{k}P_k + f_2 C_{\varepsilon 2}\bar{\rho}\varepsilon$

Table 3. $k-\acute{U}$ RANS Model.

The eddy-viscosity is defined as $\mu_t = \bar{\rho}C_\mu f_\mu \frac{k^2}{\varepsilon}$, and production of turbulent kinetic energy is,

$$P_k = \left[\mu_t\left[\nabla\vec{u} + \nabla\vec{u}^T\right] - \frac{2}{3}\left[\mu_t\left(\nabla\cdot\vec{u}\right) + \bar{\rho}k\right]\mathbf{I}\right] : \nabla\vec{u}$$

The three functions $\left(f_\mu, f_1, f_2\right)$ are part of the low Reynolds number version, taking into account the important influence of walls. It is common practice to include the turbulent kinetic with the pressure

$$\bar{P} = P + \frac{2}{3}\bar{\rho}k$$

and thus **T** is modified appropriately. In general three boundary conditions for inflow/outflow, periodic and no-slip walls will be required. At a no-slip surface the fluctuating velocity equals zero so *k*=0. No natural condition for ε_w exists and is model dependent.

1.2.2 Large eddy simulation equations

RANS equations model all of the turbulent fluctuations thus lumping all the physical processes associated with unsteady turbulent fluctuations into effective constitutive parameters such as eddy viscosity or conductivity. Higher fidelity flow analysis will also be pursued based on large eddy simulation where two assumptions are made; 1) most of the turbulent transport is carried out by the large scales which are directly computed and 2) the small (sub-grid) unresolved scales are more universal than the large scales and can be described by relatively simple eddy-viscosity models.

Consider a single constituent incompressible fluid. The sub-grid stress tensor arising in the filtered momentum equation is;

$$\tau^{sgs} = \left(\overline{\mathbf{uu}} - \bar{\mathbf{u}}\bar{\mathbf{u}}\right).$$

Similar to RANS, the sub-grid stress tensor is modeled using the Boussinesq assumption;

$$\tau^{sgs} - \frac{1}{3}\tau^{sgs}\mathbf{I} = -2\bar{\rho}\upsilon_t\bar{\mathbf{S}}$$

where the filtered strain rate tensor is defined as;

$$\bar{\mathbf{S}} = \frac{1}{2}\left[\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^T\right].$$

1.2.2.1 Smagorinsky model

The eddy viscosity will be computed using a variation of the Smagorinsky model.
The first variation contains Van Driest damping suitable for wall-bounded flows [5,6];

$$\upsilon_t = \left(C_S\left[1 - \exp\left(y^+ / A^+\right)\right]\right)^2\left|\bar{S}\right|$$

where $A^+ = 26$, $y^+ = yu_\tau / \upsilon$, $u_\tau = \sqrt{\tau_w / \bar{\rho}}$ and τ_w is the wall shear stress.

1.2.2.2 Wall adapting local eddy viscosity model

The second variation is a model called wall adapting local eddy-viscosity (WALE). The WALE model [7] contains the attractive properties that it is spatially local and the eddy-viscosity goes to zero at the wall without the aid of a damping function. The eddy-viscosity model is defined as;

$$\upsilon_t = \left(C_w \Delta\right)^2 \frac{\left(\bar{S}_{ij}^d \bar{S}_{ij}^d\right)^{3/2}}{\left(\bar{S}_{ij}\bar{S}_{ij}\right)^{5/2} + \left(\bar{S}_{ij}^d \bar{S}_{ij}^d\right)^{5/4}}$$

where the square of the deviatoric stress tensor is defined as,

$$\bar{S}_{ij}^d = \bar{S}_{ik}\bar{S}_{kj} + \bar{\Omega}_{ik}\bar{\Omega}_{kj} - \frac{1}{3}\delta_{ij}\left[\bar{S}_{mn}\bar{S}_{mn} - \bar{\Omega}_{mn}\bar{\Omega}_{mn}\right]$$

$C_w = 0.5$, and the rotation tensor is defined as; $\bar{\Omega} = \frac{1}{2}\left[\nabla\bar{\mathbf{u}} - \nabla\bar{\mathbf{u}}^T\right]$.

1.2.2.3 Sub-grid kinetic energy model

In addition to Smagorinsky's model, an eddy-viscosity model derived from the sub-grid kinetic energy [8] will be investigated. This model makes no assumption of equilibrium (i.e., production does not have to equal dissipation of sub-grid kinetic energy, $P^{sgs} \neq D^{sgs}$). In addition it provides a rational sub-grid turbulence quantity that can be used for closure of other transported quantities such as species mixing. The sub-grid kinetic energy is defined as;

$$k^{sgs} = \frac{1}{2}\left(\overline{\mathbf{u}\mathbf{u}} - \bar{\mathbf{u}}\bar{\mathbf{u}}\right).$$

The transport equation for the sub-grid kinetic energy is;

Sub-Grid Kinetic Energy	$R_k = \frac{\partial k^{sgs}}{\partial t} + \bar{\mathbf{u}}\cdot\nabla k^{sgs} - \nabla\cdot\left(\upsilon_t \nabla k^{sgs}\right) - P^{sgs} + D^{sgs}$

Table 4. Sub-grid kinetic energy model equation.

The sub-grid eddy-viscosity is defined as $\upsilon_t = C_\upsilon \Delta\left(k^{sgs}\right)^{1/2}$, production of sub-grid kinetic energy is $P^{sgs} = -C_k \tau^{sgs}\cdot\nabla\bar{u}$, and the dissipation is $D^{sgs} = C_\varepsilon\left(k^{sgs}\right)^{3/2}/\Delta$. The model constants are $C_\upsilon = 0.0854,\ C_k = 1.0,\ C_\varepsilon = 0.916$ and the grid scale is $\Delta = \left(\Delta_{x1}\Delta_{x2}\Delta_{x3}\right)^{1/3}$. At a no-slip surface, $k^{sgs} = 0$. Similar to Smagorinski's model, Van Driest damping is also required by this model.

2. Spatial and temporal discretization

In this section we very briefly describe the stabilized FE methods used for discretization of the Navier-Stokes equations with coupled transport. The governing PDEs for the flow and transport system are presented in Table 1-4. Our stabilized FE formulation is capable of handling incompressible, low Mach number, variable density (temperature and chemical species dependent), and low speed compressible flows. This flexibility is enabled by the fully-implicit time integration and fully-coupled nonlinear solver technology that is described below.

2.1 Stabilized FE discretization

Consistently stabilized finite element methods [9,10] are constructed in the current formulation. Table 5 presents the associated FE weak form for the PDEs presented in Table 1-4. This system employs equal-order interpolation, which allows one to simplify the data structures of a parallel unstructured FE code and the linear algebra interface for iterative solution methods [11-13]. To improve stability for highly convected flows we employ discontinuity-capturing operators that provide additional crosswind diffusion to supplement the natural streamline diffusion contribution of the GLS stabilization. The resulting finite element formulation decreases numerical oscillations (compared with standard SUPG schemes) and allows for stable and accurate finite element solutions when the cell Reynolds, Re_c, and thermal energy and mass transport Peclet numbers, Pe_c, are greater than one. The stabilized FE formulation described above has been shown numerically to be 2nd order accurate in space and time on smooth solutions when combined with an appropriate semi-discrete time discretization (e.g. Trapezoidal rule, BDF2, or Midpoint rule).

Governing Equation	Stabilized FE Weak Form Residual Equation for Low Mach Number Flow
Momentum	$F_{m,i} = \int_\Omega \Phi R_{m,i}\, d\Omega + \sum_e \int_{\Omega_e} \tau_m (\mathbf{u}\cdot\nabla\Phi) R_{m,i}\, d\Omega + \sum_e \int_{\Omega_e} \nu_{m,i} \nabla\Phi \cdot \Theta \nabla \mathbf{u}_i\, d\Omega$
Continuity	$F_p = \int_\Omega \Phi R_p\, d\Omega + \sum_e \int_{\Omega_e} \rho \tau_m \nabla\Phi \cdot \mathbf{R_m}\, d\Omega$
Energy	$F_T = \int_\Omega \Phi R_T\, d\Omega + \sum_e \int_{\Omega_e} \rho \hat{C}_p \tau_T (\mathbf{u}\cdot\nabla\Phi) R_T\, d\Omega + \sum_e \int_{\Omega_e} \nu_T \nabla\Phi \cdot \Theta \nabla T\, d\Omega$
Spalart-Allmaras	$F_{SA} = \int_\Omega \Phi R_{SA}\, d\Omega + \sum_e \int_{\Omega_e} \rho \tau_{SA} (\mathbf{u}\cdot\nabla\Phi) R_{SA}\, d\Omega + \sum_e \int_{\Omega_e} \nu_{SA} \nabla\Phi \cdot \Theta \nabla \hat{\nu}\, d\Omega$

Table 5. Stabilized FE weak form residuals for the Spalart-Allmaras RANS model. The first term is the Galerkin term, followed by the SUPG term and the discontinuity capturing term. Here the Θ operator is a cross-stream oriented tensor, that adds diffusion in the cross-stream direction, that is orthogonal to the SUPG contribution.

2.2 Preconditioned Newton-Krylov method

The result of a fully-implicit or direct-to-steady-state solution technique is the construction of very large-scale, coupled highly nonlinear algebraic system(s) that must be solved. Therefore, these techniques place a heavy burden on both the nonlinear and linear solvers and require robust, scalable, and efficient nonlinear solution methods. In the present code, Newton-based iterative nonlinear solvers [14] are employed to solve the nonlinear systems that result in this application. These solvers can exhibit quadratic convergence rates independently of the problem size when sufficiently robust linear solvers are available. For the latter, we employ Krylov iterative techniques. A Newton-Krylov (NK) method [15,16] is an implementation of Newton's method in which a Krylov iterative solution technique is used to approximately solve the linear systems, $\mathbf{J}_k\mathbf{s}_{k+1} = -\mathbf{F}_k$, that are generated at each step of Newton's method. The Jacobian matrix, $\mathbf{J}_k$, that is used for the Jacobian-vector products in the Krylov solvers, and as the basis for computing the preconditioners described here, is developed from automatic differentiation (AD) techniques. These methods are applied to the programmed functions representing the weak form residuals outlined in Table 5.

2.3 Parallel preconditioning methods

For the considered class of linear systems described above, convergence is only achieved with preconditioning due to ill-conditioning in the underlying matrix equations [17]. Traditionally, Schwarz domain decomposition (DD) with block incomplete factorization, ILU(k) has been used to precondition the systems. However, these techniques do not scale well as the problem size is increased. In fact, the number of iterations required to solve the linear system increases as the number of processors is increased. Instead, algebraic multi-grid (AMG) solution methods will be used. These are significantly easier to implement and integrate within complicated unstructured simulation codes compared with traditional geometric multi-grid methods, which require coarse grids [18,12,19]. The advantage of AMG is that the iteration count does not increase nearly as much, as the number of processors increased, compared to traditional preconditioners. In addition, approximate block factorization (ABF) [20-22] and physics-based approaches [23] are used to take advantage of small time scale transients in a way that improves convergence of the linear solvers. By employing AMG and ABF techniques, fully implicit methods applied to small time scale transient flows becomes much more tractable than previous generation stabilized FE formulations.

3. Results included in final draft

Results that contribute to the two major themes in this paper will be presented in the final draft. One theme is how well URANS and LES methodologies predict the flow characteristics in a 3x3 rod bundle reactor core incompressible, single-phase adiabatic prototype model. While using URANS is desirable from a cost stand point, in general, it has been accepted that LES produces higher fidelity solutions especially for anisotropic unsteady turbulent flows. The relative cost of URANS vs. LES and the relative fidelity of the two solution methods will be investigated and reported on in the final version of this paper.

The second theme has to do with how well the linear equation system solver preconditioners perform for high Reynolds number transient flows. Various preconditioning techniques

developed specifically for this flow regime will be compared and reported on. These results will provide important data to be used on future simulations of larger rod bundles.

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