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A Newton solution for the Superhomogenization method: The PJFNK-SPH

Javier Ortensi [a,*], Yaqi Wang [a], Alexandre Laurier [b], Sebastian Schunert [a], Alain Hébert [b], Mark DeHart [a]

[a] Idaho National Laboratory, 2525 N. Fremont Ave., Idaho Falls, ID 83401, USA
[b] École Polytechnique de Montréal, 2900 Boulevard Edouard-Montpetit, Montréal, QC H3T 1J4, Canada

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ABSTRACT

This work presents two novel topics regarding the Superhomogenization method: 1) the formalism for the implementation of the method with the linear Boltzmann Transport Equation, and 2) a Newton algorithm for the solution of the nonlinear problem that arises from the method. These new ideas have been implemented in a continuous finite element discretization in the MAMMOTH reactor physics application. The traditional solution strategy for this nonlinear problem uses a Picard, fixed-point iterative process whereas the new implementation relies on MOOSE's Preconditioned Jacobian-Free Newton Krylov method to allow for a direct solution. The PJFNK-SPH can converge problems that were either intractable or very difficult to converge with the traditional iterative approach, including geometries with reflectors and vacuum boundary conditions. This is partly due to the underlying Scalable Nonlinear Equations Solvers in PETSc, which are integral to MOOSE and offer Newton damping, line search and trust region methods. The PJFNK-SPH has been implemented and tested for various discretizations of the transport equation included in the Rattlesnake transport solver. Speedups of five times for diffusion and ten to fifteen times for transport were obtained when compared to the traditional Picard approach. The three test problems cover a wide range of applications including a standard Pressurized Water Reactor lattice with control rods, a Transient Reactor Test facility control rod supercell and a prototype fast-thermal reactor. The reference solutions and initial cross sections were obtained from the Serpent 2 Monte Carlo code. The SPH-corrected cross sections yield eigenvalues that are near exact, relative to reference solutions, for reflected geometries, even with reflector regions. In geometries with vacuum boundary conditions the accuracy is problem dependent and solutions can be within a few to a few hundred pcm. The root-mean-square error in the power distribution is below 0.8% of the reference Monte Carlo. There is little benefit from SPH-corrected transport in typical scoping calculations, but for more detailed analyses it can yield superior convergence of the solution in some of the test problems. This PJFNK-SPH approach is currently being used in the modeling of the Transient Test Reactor at Idaho National Laboratory, where full reactor core SPH-corrected cross sections are employed to reduce the homogenization errors in transient or multi-physics calculations. This base implementation of the PJFNK-SPH provides an extremely robust solver and a springboard to further improve the Superhomogenization method in order to better preserve neutron currents, one of the primary deficiencies of the method.

1. Introduction

Idaho National Laboratory (INL) has developed a high fidelity, strongly coupled multi-physics modeling capability under the Multi-physics Object Oriented Simulation Environment (MOOSE) framework (Gaston et al., 2009). MAMMOTH (Gleicher et al., 2014) is a MOOSE-based reactor physics application that couples Rattlesnake (radiation transport) (Wang, 2013), BISON (fuel performance) (Williamson et al., 2012), RELAP-7 (thermal-fluids) (Berry and Peterson, 2014), etc. Rattlesnake solves the steady-state, transient and k-eigenvalue problems for the multi-group radiation transport equations, the linear Boltzmann Transport Equation (BTE) discretized with the multigroup approximation for the energy variable. There are a number of different transport schemes available in Rattlesnake including self-adjoint angular flux (SAAF) formulation, the least squares formulation (LS) and the first order transport formulation. Rattlesnake also has a number of angular discretization schemes including spherical harmonics expansion (P_N), discrete ordinates (S_N) and diffusion.

* Corresponding author.
E-mail address: javier.ortensi@inl.gov (J. Ortensi).

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There are continuous and discontinuous Finite Element Methods (FEM) for solving the P_N, S_N, and diffusion angular representation. Currently, the most tested and optimized solvers use the continuous FEM representation.

Most nuclear reactors are still too complex to allow high resolution modeling in every instance or there exist other constraints, e.g. run time for transient calculations, thus rendering detailed transport calculations infeasible. The method of choice for reducing the model complexity and allowing a reasonable representation without requiring too high a computational cost is the spatial homogenization of regions. Unfortunately, this spatial homogenization usually incurs errors that stem from the loss of information and fine details. There are currently two widely used homogenization techniques that aim to properly reproduce key quantities obtained from detailed computations of heterogeneous reactor regions. Both of these techniques are based on equivalence theory which states that, for each macro region in the homogenized reactor calculation, the averaged fluxes and reaction rates are to be in agreement with the heterogenous calculation. A literature search on various equivalence techniques can be found in the thesis that this work extends (Laurier, 2016).

The first method, expanding on equivalence theory, is called Generalized Equivalence Theory (GET) (Smith, 1986). Smith added another degree of freedom to the equations to allow the conservation of more than just averaged reaction rates and fluxes. This new parameter, called "discontinuity factor" (DF), allows for a better approximation of the neutron flux or currents at the boundaries. Although DFs produce good results in highly heterogeneous assemblies, the computational memory needed to do so is high, since a DF factor must be calculated and stored for every cell surface. Additionally, it requires a discontinuous method, which further demands evaluations at the cell surfaces. This heavy memory usage makes the use of DF difficult for three-dimensional pin-by-pin calculations. This equivalence procedure also has to explicitly take into account each discontinuity factor when solving the neutron transport equation over the full core whereas other methods allow for simpler modifications. A limiting aspect of this method arises from the availability of solvers with the capability of using discontinuous methods, which, as previously mentioned, are not yet well optimized within the Rattlesnake application.

The second widely used homogenization procedure, and the focus of this work, is called the Superhomogenisation (SPH) method. First described by Kavenoky et al. (1978) and later generalized by Hébert (1981), Hébert and Benoist (1991), Hébert (1993), Hébert and Mathonnière (1993), it introduces a new homogenization parameter, the SPH factor, to correct homogenized cross section errors. These SPH factors are applied to each averaged cross section to exactly reproduce the reaction rates from the heterogeneous calculation. Thus, for each macro region and energy group there is a unique SPH factor that is calculated, applied and does not need to be stored separately. This standard solution algorithm for obtaining the SPH factors is a fixed-point iterative method, which takes place between the main transport solver and the cross section modification step and does not require the modification of the already available full-core solvers to use SPH-corrected cross sections. One of the known shortcomings of the SPH method resides in its inability to conserve the neutron leakage. This is mainly due to the fact that the SPH method does not include enough degrees of freedom to preserve the currents between cells. A test illustrating this fact is included in Section 3.1.

In summary, the advantages of the SPH method over DFs are:

- simple implementation dealing with volumetric quantities,
- applicable to both continuous and discontinuous FEM,
- lower computational burden (no need to evaluate fluxes at the interfaces) and
- small data requirements (1 floating point per energy group per macro region).

The disadvantages of the SPH method over DFs are:

- does not produce an exact balance in geometries with reflectors or void boundary conditions and
- does not conserve currents (i.e. leakage) at the macro region interfaces.

Due to the need to implement an equivalence procedure in the continuous FEM solvers the SPH method is currently the best candidate. Since the transport systems in Rattlesnake are well modularized it was quite simple to implement the SPH procedure for a variety of solvers with minimal development effort. Therefore, the SPH procedure is now available in the continuous diffusion, SAAF-P_N and SAAF-S_N solvers.

The focus of this work is the preparation of SPH-corrected cross sections for transient simulations from complete analysis geometries and not in performing local lattice SPH corrections for assemblies in the traditional two-step analysis process (lattice-full core). This need is driven by the modeling and simulation of the Transient Reactor Test Facility (TREAT) (Ortensi et al., 2016) at INL. The current approach employs full core steady state Serpent Monte Carlo (Leppänen, 2015) models to generate cross sections. This is followed with Rattlesnake SPH calculations to prepare an SPH-corrected database later used in MAMMOTH transient simulations. Therefore, the principal interest of this work is to introduce the benefits of using a Newton Method for the SPH procedure and to investigate if there is a clear advantage to using SPH-corrected transport over SPH-corrected diffusion.

2. Methodology

2.1. The SPH equations

The Superhomogenisation (SPH) procedure is a cross section correction method that aims to preserve the reaction rates, leakage and eigenvalue within macro regions obtained through a homogeneous calculation with respect to a reference heterogeneous problem (Hébert, 1993). The correction is applied to reduce the error that originates from spatial homogenization, which modifies the physics of the problem. The SPH corrected cross sections are defined as the product of the reference cross section in macro region $m = 1, \ldots, M$ in energy group $g = 1, \ldots, G$ with its respective SPH factor $\mu_{m,g}$. There exists a unique SPH factor for each macro region m and energy group g such that the reaction rate in these regions is preserved:

$$\Sigma_{m,g} = \mu_{m,g}\Sigma^{ref}_{m,g} \tag{1}$$

In Eq. 1, the superscript "ref" represents the cross section value obtained using the condensation and homogenization process, but without applying the correction.

By definition of the SPH correction, the average reaction rate $\tau_{m,g}$ is to be preserved:

$$\tau^{ref}_{m,g} = \tau_{m,g} = \Sigma_{m,g}\phi_{m,g} = \Sigma^{ref}_{m,g}\phi^{ref}_{m,g} \tag{2}$$

where

$\phi^{ref}_{m,g}$ = reference heterogeneous flux in macro region m and group g

$\phi_{m,g}$ = homogeneous flux in macro region m and group g

$$\tau_{m,g} = \mu_{m,g}\Sigma^{ref}_{m,g}\phi_{m,g} = \Sigma^{ref}_{m,g}\phi^{ref}_{m,g} \tag{3}$$

from which the SPH factors are defined: