Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)
Monterey, California, April 15-19, 2007, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

GOAL-ORIENTED *hp*-MESH ADAPTATION FOR 1-D MULTIGROUP DIFFUSION EQUATIONS

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ABSTRACT

We propose and test a fully automated, goal-oriented *hp*-adaptivity refinement strategy for the multigroup diffusion equations. This method combines the standard *hp*-adaptation technique with a goal-oriented adaptivity based on the simultaneous solution of an adjoint problem.

Key Words: goal-oriented mesh adaptation, *hp*-refinement, multigroup diffusion.

1. INTRODUCTION

Computing highly accurate and **converged** solutions of the neutron balance equation in an automated and adaptive fashion is a challenging and important task. The issue of obtaining a solution converged to a desired (i.e., user prescribed) tolerance is seldom addressed. Using "brute force" uniform mesh refinement to answer this issue is not a credible remedy because (1) this process soon comes to a halt due to the enormous increase in the number of unknowns, and, (2) it does not guarantee that a solution has been reached within a prescribed tolerance.

The research presented here is a continuation of the study of a fully automated *hp* mesh refinement technique for the multigroup diffusion equations. One of the key advantages of this technique is that it does not require the use of any a-priori knowledge about the solution in order to estimate errors in the numerical solutions and automatically adapt the mesh to reduce these errors. This technique achieves exponential convergence rates and delivers optimal meshes. In this previous study, we implemented *hp*-refinement algorithms for the multigroup diffusion equations [1,2]. These algorithms assess the local errors, for each energy group, and adaptively refine the mesh only in areas where it is needed. A different mesh per energy group was utilized in order to follow the physics as closely as needed and to minimize the CPU and memory cost of mesh adaptation. These algorithms yield numerical solutions where the error was guaranteed to be less than the user specified tolerance in every mesh of the domain. This is achieved by bulk chasing the mesh cells with the largest errors, hence naturally producing an equal distribution of the error in the final and converged mesh.

Even though such adaptive refinement techniques made a sensible use of resources (both in CPU and memory), a highly accurate solution in every mesh cell of the computational domain may not be needed from a practical engineering point of view. Moreover, the ultimate answer may not be the solution itself but rather a functional of the solution, such as a reaction rate integrated over a given volume, or a particle flux or current at a given point, for a given energy group. This motivates

improvements to the previous algorithms in order to bring together (1) the need for accurate solution in quantities of interest and (2) *hp*-adaptivity, hereby proposing goal-oriented *hp*-adaptivity.

In section 2, we briefly review the basics of *hp*-strategy applied to multigroup equations. In section 3, we introduce the adjoint based formalism for goal-oriented adaptivity. The next section presents our results.

2. A REVIEW OF STANDARD *hp*-ADAPTIVITY APPLIED TO THE MULTIGROUP EQUATIONS

In the last decade, the theory of a posteriori error estimations [3] has matured and allows the measure, control and minimization of approximation errors. In this theory, the computed solution itself is used to provide inexpensively point-wise error estimations. The greatest advantages of the *hp*-strategy [4,5,6] is that it does not need any beforehand information about singularities or steep gradients of the solution and that it fully automatically delivers exponential convergence rates (in terms of number of unknowns). The strategy does not use any explicit error estimates to guide the *hp*-refinements; instead, an approximate error function is recovered from a suitable "reference" solution. The reference solution, obtained on a finer *hp*-mesh, is also an approximation of the exact solution but it is substantially more accurate than the approximation on the coarse mesh. The sequence of optimal *hp*-meshes is obtained by minimizing the appropriate interpolation error in each step of the mesh adaptation.

2.1. *hp*-mesh adaptation strategy

In the framework of finite element methods, not only can we split or coarsen a mesh locally (*h*-refinement) but we can also vary locally the polynomial degree of the expansion basis (*p*-refinement, where *p* denotes the degree of the polynomial approximation). The two approaches can be combined into what is called *hp*-refinement. For neutronics calculations, *h*-refinement [7] and *p*-refinement [8,9] have been previously investigated. Nonetheless, neither the *h*-method nor the *p*-method yield optimal convergence rates [10]: *h*-refinement is advised in regions where the solution is not smooth, whereas *p*-refinement (akin to spectral methods) should be used in regions where the solution is smooth. In order to obtain a mesh that yields exponential convergence, mesh cells chosen for refinement must either undergo an *h*-refinement or a *p*-refinement, depending on which process produces the greatest error reduction. This choice leads to competitive *hp*-adaptivity.

2.2. Multigroup issues related to *hp*-adaptivity

hp-strategies found in the literature usually deal with only one equation. The multigroup approximation in neutron conservation laws leads to a series of coupled equations (due to scattering and fission events which transfer neutrons from a group to another group). Solving the multigroup equations on group-dependent meshes follows the nature of the problem and minimize the usage of CPU and memory but requires spatial projections and interpolations between source terms of different energy groups for a given adaptivity phase. It turns out that projection and interpolation operations are not needed; the only matter at hand is the computation of scattering and fission mass matrices, where shape functions and test functions are polynomials of various orders defined on non-matching cells. A simple adaptive integration method has been used to compute these mass matrices. [1,2]

3. GOAL-ORIENTED *hp*-ADAPTIVITY FOR THE MULTIGROUP EQUATIONS

During the past decade [11], goal-oriented adaptivity for PDE's has been the topic of various methodologies. In comparison with standard mesh adaptivity, which aims at minimizing the residual of the approximate solution (i.e., equi-distribution of the errors), goal-oriented refinement aims at controlling specific features of the solved problems (the quantities of interest) in order to reach accurate resolution in these quantities with significantly fewer degrees of freedom than the standard *hp*-adaptation.

The following equations are examples of quantities of interest:

- a reaction rate in a given volume *V*: $I(\phi) = \sum_{g=1}^{G} \int_V \Sigma_{g,d}(x)\phi_g(x)dx$ where the subscript *d* represents a specific reaction type;
- a current at a point x_0 for a given group *g*: $I(\phi) = J_g(x_0)$;
- a flux at a point x_0 for a given group *g*: $I(\phi) = \phi_g(x_0)$.

The error in the quantities of interest between the fine (reference) *hp* mesh and coarse *hp* mesh is, by definition, given by

$$e_{hp} = \left| I(\phi) - I(\phi_{hp}) \right| = \left| b(\phi - \phi_{hp}, \phi^* - \phi^*_{hp}) \right| \qquad (1),$$

where Galerkin's orthogonality property has been used. *b* is the bilinear form representing the variational diffusion problem. Following the same error estimation derivation used for standard *hp*-adaptivity, but modifying it for the purpose of goal-oriented adaptivity, we arrive at the following formula for the goal-oriented error estimates:

$$e_{hp} \le C \sum_{g=1}^{G} \sum_{K_g} \mu_{g,k} \quad \text{where} \quad \mu_{g,k} = \left\| \phi_{g,ref,k} - \prod_{h,p_{g,K}} \phi_{g,ref,k} \right\|_1 \left\| \phi^*_{g,ref,k} - \prod_{h,p_{g,K}} \phi^*_{g,ref,k} \right\|_1 \qquad (2)$$

where the continuity and coercivity properties of the bilinear form *b* has been invoked and the H^1 norm is employed in the error estimates. ϕ^* is the adjoint flux, solution of the adjoint problem, whose source term depends on the quantity of interest *per se*. Goal-oriented calculations hence require both the direct and adjoint fluxes to proceed. Although this may seem as a drawback compared with standard *hp*-adaptation, the number of unknowns in goal-oriented calculations is significantly smaller. The goal-oriented adaptivity process then proceeds as with the standard *hp*-techniques, using the error estimator $\mu_{g,k}$ to chase the bulk of the error and refine the meshes where needed. The main difference with standard *hp*-adaptivity is that $\mu_{g,k}$ embeds the adjoint solution (neutron importance to due to a given adjoint source). Some adjoint sources and their associated quantities of interest are given below:

Quantity of interest	Adjoint source
Pointwise flux $\phi_g(x_0)$	$s^*_{ext,g'} = \delta(x-x_0)\delta(g'-g)$
Reaction rate for reaction R in group g for $x \in [x_1; x_2]$	$s^*_{ext,g'}(x) = \Sigma_{g,R}(x)\delta(g'-g)$ for $x_1 \le x \le x_2$, 0 otherwise
Pointwise current $J_g(x_0)$	$s^*_{ext,g'} = \frac{d}{dx}(D_g(x)\delta(x-x_0))\delta(g'-g)$

4. RESULTS

We present here the results of goal-oriented calculations for 1-D, 2-g diffusion problems.

4.1 Test #1: quantity of interest as the thermal flux within a specific spatial zone.

In this goal-oriented test, the flux in a particular region of the problem is the quantity of interest. The geometry of this problem consists in 7 100-cm thick zones, whose material numbers are arranged as follows: 1-2-3-2-3-3-2. The material cross sections are given in Table I, and the strength of the fast group source is, per spatial zone, 0.0-1.5-1.8-1.5-1.8-1.8-1.5 $cm^{-3}sec^{-1}$. Zero-flux boundary conditions hold at both extremities. Fig. 1 shows the fast and thermal flux distributions, converged to a user-defined tolerance of 10^{-5}% using the standard *hp*-technique.

Table I. Material properties for the Test Problem #1.

Material #	D^1 (cm)	D^2 (cm)	Σ_r^1 (cm^{-1})	Σ_r^2 (cm^{-1})	$\Sigma_s^{1\to2}$ (cm^{-1})	$\nu\Sigma_f^1$ (cm^{-1})	$\nu\Sigma_f^2$ (cm^{-1})
1	1.2	0.4	0.03	0.1	0.02	0.005	0.1
2	1.2	0.4	0.03	0.2	0.015	0.0075	0.1
3	1.2	0.4	0.03	0.25	0.015	0.0075	0.1

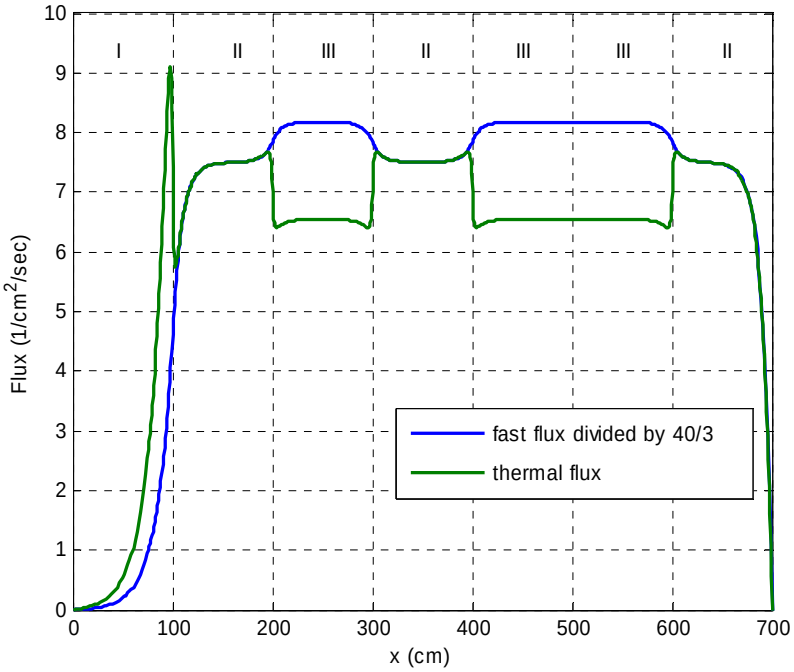

Fig. 1. Fast and Thermal Flux distributions (tolerance = 10^{-5}%), Test Problem #1.

For the goal-oriented calculation, the region of interest extends from 100 cm to 300 cm. Figures 2, 3, and 4 present the goal-oriented converged direct flux distribution, the direct flux mesh, and the adjoint flux distribution, respectively. We can clearly see that, in the region of interest, the flux is properly computed and is identical to the results of Fig. 1. The effect of the user-defined tolerance is also in Fig. 2, where the results for tolerances of 1%, 0.1%, and 10^{-3}% are presented. Outside of that region of interest, the solution becomes inaccurate and, finally, meaningless. The meshes, used to compute the direct fluxes with a tolerance of 10^{-3}%, are given in Fig. 3. Fig. 3 shows that the elements and the polynomial order are concentrated in the vicinity of the region of interest. Because the error estimate utilizes an error distribution weighted by the adjoint flux, elements are preferentially refined where the adjoint flux is significant. The adjoint flux is shown in Fig. 4.

The number of unknowns for the goal-oriented calculation was about 65% smaller than for the standard *hp*-technique. With an even further spatially restricted quantity of interest, the number of unknowns in the goal-oriented calculation would have been even smaller.

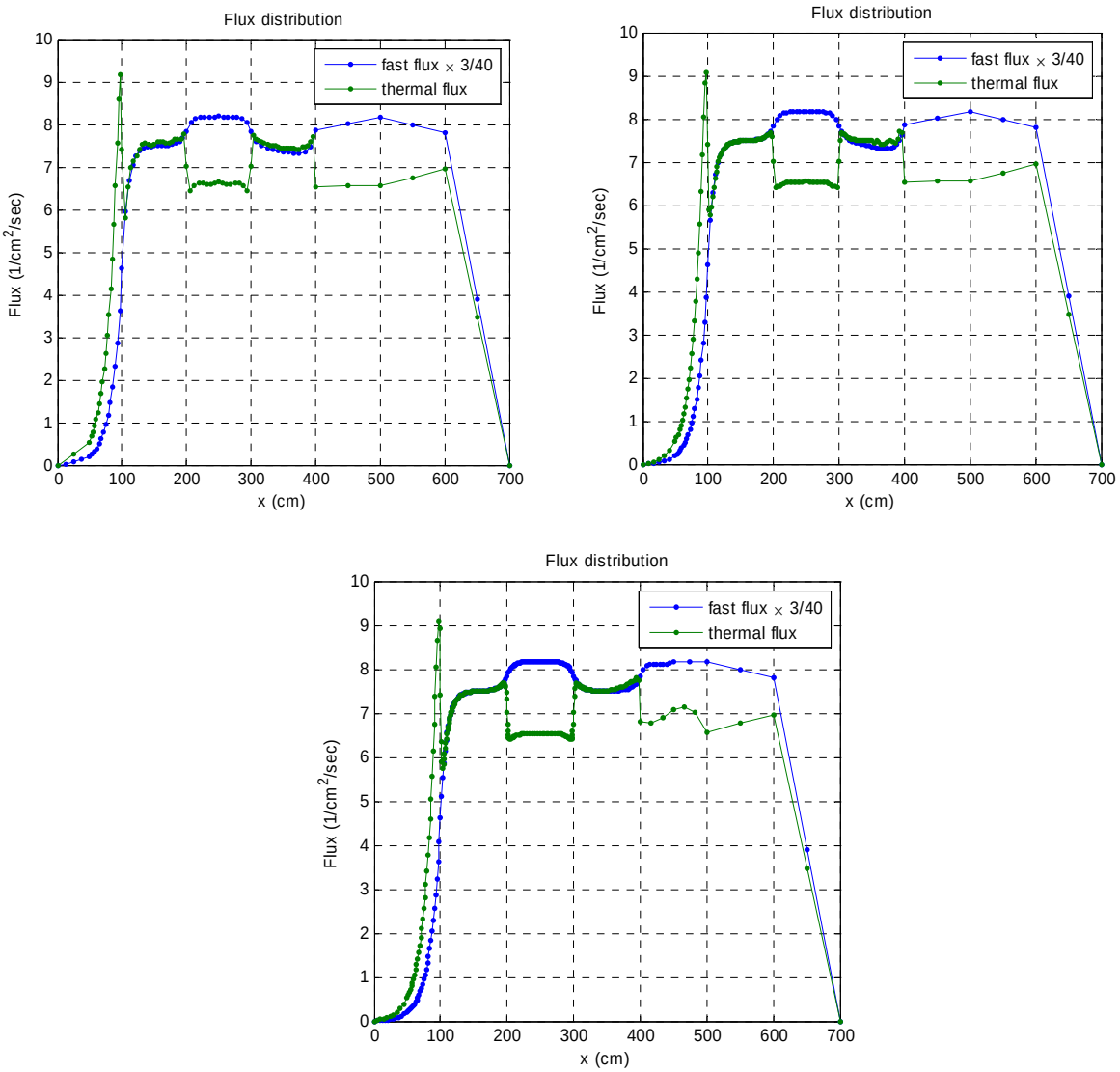

Fig. 2. Flux distributions, goal-oriented calculation, flux as quantity of interest in $100 \leq x \leq 300$ (Model Problem B1). Tolerances used: top-left = 1%; top-right = 0.1%; bottom = 0.001%.

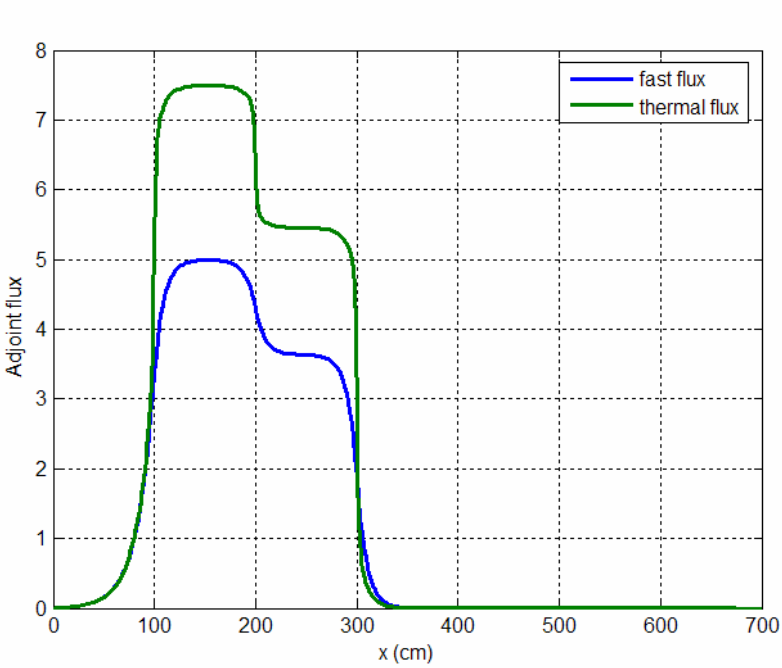

Fig. 3. Adjoint flux distributions, goal-oriented calculation, flux as quantity of interest in $100 \le x \le 300$ (Test Problem #1).

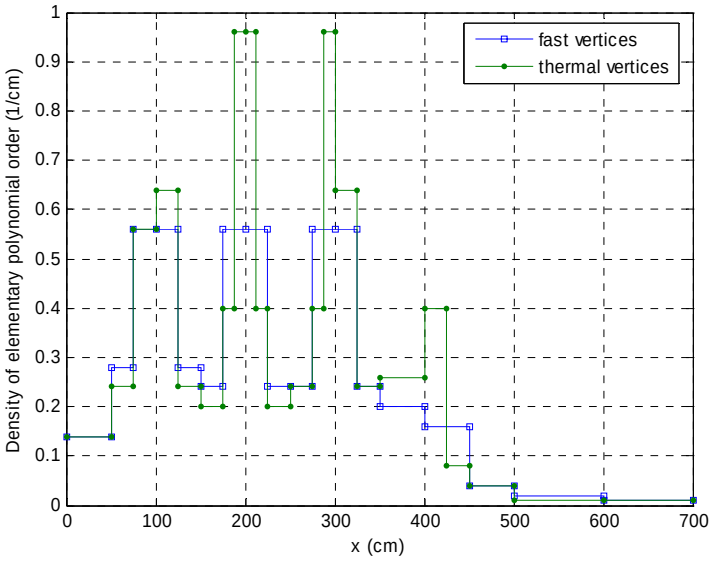

Fig. 4. Mesh distribution. Goal-oriented calculation, flux as quantity of interest in $100 \le x \le 300$ (Test Problem #1).

4.2 Tests #2 and #3: quantity of interest as the thermal flux and thermal current at a specific location.

For these tests, we once again use the configuration of the Test Problem #1. In that problem, we observed a sharp thermal flux gradient in the vicinity of $x_0 = 100\,\text{cm}$. For these tests, we selected as

quantities of interest the point-wise thermal flux (Test Problem #2) and the point-wise thermal net current (Test Problem #3) at that location. Fig. 5 depicts the converged direct and adjoint fluxes used to calculate the thermal flux at x_0 within a tolerance of 1%. The adjoint fluxes are only significant in the vicinity of x_0. Fig. 6 depicts the converged direct and adjoint fluxes used to calculate the thermal net current at x_0 within a tolerance of 1%. Again, the adjoint fluxes are only significant in the vicinity of x_0. Depending on the sign of the load vector for the adjoint equation, the adjoint flux can be positive or negative around x_0.

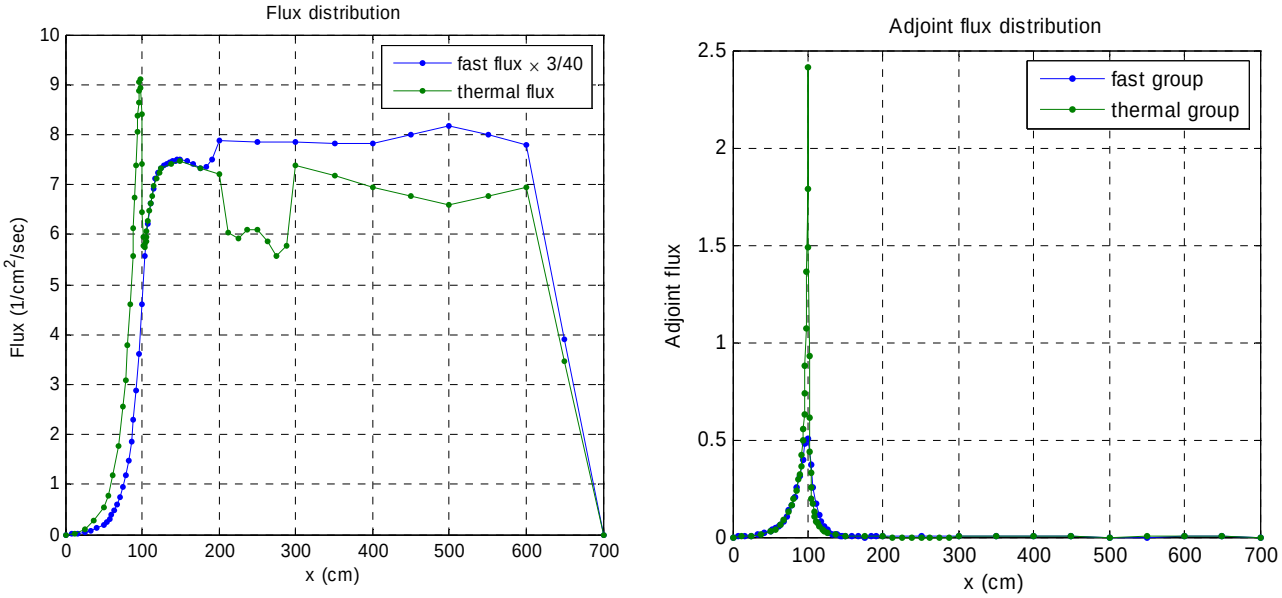

Fig. 5. Flux distribution, goal-oriented calculation, flux as quantity of interest at $x = 100$, tolerance = 1% (Test Problem #2). Left = direct flux, right= adjoint flux

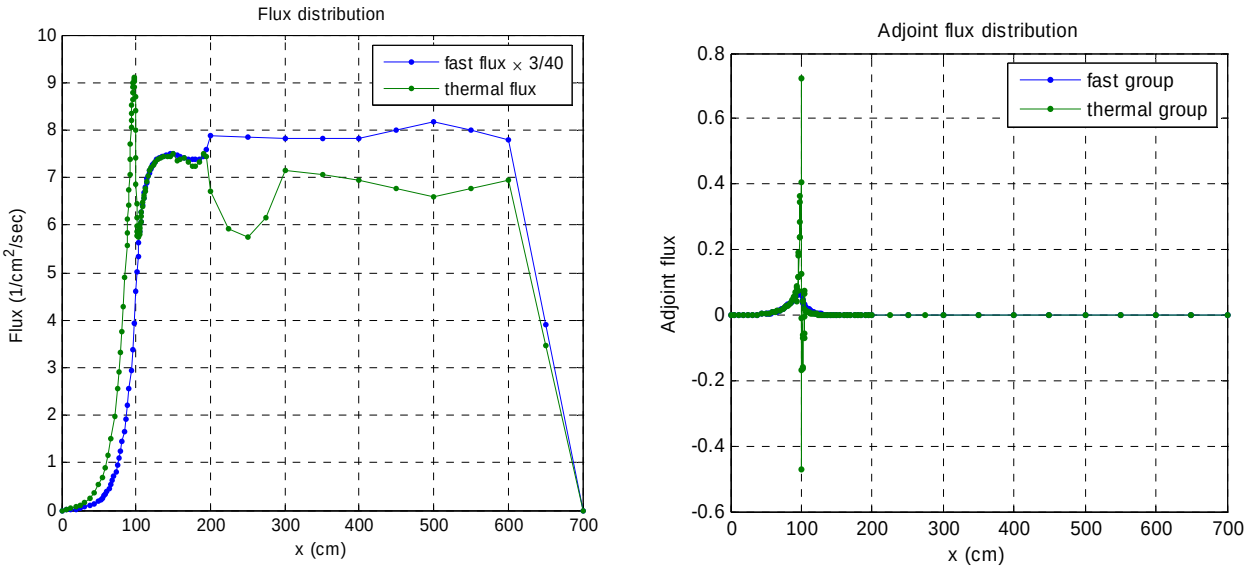

Fig. 6. Flux distribution, goal-oriented calculation, current as quantity of interest at $x = 100$, tolerance = 1% (Test Problem #3). Left = direct flux, right= adjoint flux.

5. CONCLUSIONS

Our work applied two powerful numerical techniques to the multigroup diffusion equation: *hp*-mesh adaptivity and goal-oriented simulation based on the adjoint problem. A numerical solution can be attained to a user prescribed tolerance with exponential rates of convergence. Even though goal-oriented simulations require both the direct and the adjoint flux to be solved, the number of unknowns is reduced in comparison of standard *hp*-refinement techniques because the meshes are only refined in regions of interest.

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