International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

SPATIAL ADAPTIVITY FOR TIME-DEPENDENT DIFFUSION PROBLEMS

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ABSTRACT

A new scheme for the efficient application of spatial adaptivity to time-dependent problems has been derived. Specifically, we avoided having recourse to several consecutive mesh adaptations per time step, but rather derived a criterion to allow the same spatial mesh to be employed for several time steps before performing a new mesh adaptation, thus reducing the computational cost while preserving the quality of the numerical solution.

Key Words: mesh adaptivity, mesh adaptation, time-dependent problems, finite-element.

1. INTRODUCTION

In recent years, mesh adaptivity for steady-state problems has become increasingly popular in the nuclear science and engineering community [1–7]. Nonetheless, little attention has been paid to spatial mesh adaptation for time-dependent problems. However, the promise of reducing the computational burden of multi-dimension time-dependent simulations thanks to spatial adaptivity is an important and exciting challenge. During transients, physical phenomena may propagate in the computational domain (e.g., wave propagation, change in boundary layers, etc) and regions of the domain where the mesh resolution was initially fine enough may require further refinement as the transient proceeds; similarly, a physical phenomenon may exit a finely refined region of the domain, allowing the said region to be coarsened. It is clear that a single adapted or uniform spatial mesh, valid for all times, may very well be impractical or suboptimal for many simulations. In this paper, we propose a mesh adaptivity technique that reduces some of the work associated with spatial adaptivity for transients.

2. SPATIAL MESH ADAPTIVITY IN TIME-DEPENDENT PROBLEMS

One of the concerns related to mesh adaptivity in time is that the adapted mesh must be appropriate for the entire time interval $[t_i\,;\,t_{i+1}]$ in order to capture all relevant spatial physical phenomena [8]. For simplicity, let us consider the diffusion approximation for photon conservation:

$$\frac{1}{c}\frac{\partial \Phi}{\partial t} = \boldsymbol{\nabla}\cdot D\boldsymbol{\nabla}\Phi - \Sigma_a\Phi + S \tag{1}$$

With backward Euler time differencing over $[t_i\,;\,t_{i+1}]$ and spatial finite element discretization, we arrive at a linear system of the form

$$(M - c\Delta t A)\Phi^{i+1} = M^{*}\Phi^{i} + f \tag{2}$$

where A represent the stiffness and mass matrix of the steady state equation, f is the right-hand-side vector containing the external source term, and M and M^* are mass matrices (when Φ^{i+1} and Φ^i are obtained on the same mesh, these 2 matrices are equal). Now suppose that the solution at the beginning of the time step t_i results from a mesh adaptation procedure and has been converged to a certain given accuracy on mesh $\mathcal{M}^i_{cv}$. The solution at the end of the time step t_{i+1} may require a different mesh, to be denoted by $\mathcal{M}^{i+1}_m$, where m-th is the mesh iteration index (with subscript m to be replaced by cv upon convergence). In mesh adaptation, the fraction of cells to be coarsened is, in practice, always smaller than the fraction of cells selected for refinement during one iteration of mesh adaption. Thus, initializing the mesh at the end of the time step using the mesh from the beginning of the time step (i.e., $\mathcal{M}^{i+1}_0 = \mathcal{M}^i_{cv}$) will likely increase the number of spatial unknowns as the simulation proceeds in time. A simple rule of the thumb would be to initialize the new mesh with $\mathcal{M}^{i+1}_0 = \mathcal{M}^i_{cv-5}$, i.e., not with the converged mesh obtained previously but with an *almost* converged mesh (the number 5 is purely indicative and heuristic). These two approaches, briefly discussed above, would still require at each mesh iteration m that a new mass matrix M^* be computed since it represents the projection of Φ^i (obtained on $\mathcal{M}^i_{cv}$) onto the current mesh $\mathcal{M}^{i+1}_m$. The drawbacks of these approaches include

1. many projections of the solution at the initial time step onto meshes at the end of the time step (matrix M^*),
2. a lack of rational for initializing the mesh to be used for the solution at the end of the time step, and
3. a lack of criterion to decide when a solution has not changed enough over time to require a new mesh.

Therefore, we decided to tackle the issue of mesh adaptivity in time with a new perspective, described below.
In order to minimize the number of times the projection matrix M^* is constructed, and to better understand when a mesh needs to be changed (refined or coarsened), we devised the following procedure which aims at keeping the same spatial mesh for as many time intervals as possible:

0. Let t_i to the beginning time stamp, from which we will seek ℓ time intervals that can accommodate the same spatial mesh with acceptable (low) error. The end time stamp will be $t_{i+\ell}$. Note that the solution at time t_i has been previously computed and reside on mesh $\mathcal{M}^i_{cv}$ and a projection matrix M^* will be needed over the time span from t_{i+1} until $t_{i+\ell}$. We start by letting $\ell = 1$.
1. At time $t_{i+\ell}$, set the mesh to be $\mathcal{M}^{i+\ell}_{m=0} = \mathcal{M}_0$, where $\mathcal{M}_0$ is a user-supplied (coarse and uniform) mesh.

2. Compute the solution $\Phi^{i+\ell}$ as well as the spatial error estimator $\boldsymbol{e}_{i+\ell}$ (for more details about error estimators, please refer to both the references cited in the introduction and a description to follow.)

3. *Without* mesh adaptation, advance to the next time time and compute $\Phi^{i+\ell+1}$ and $\boldsymbol{e}_{i+\ell+1}$. Verify how much the spatial error has evolved between $t^{i+\ell}$ and $t^{i+\ell+1}$ using the following formula

$$cos(\theta_\ell) = \frac{\boldsymbol{e}_{i+\ell} \cdot \boldsymbol{e}_{i+\ell+1}}{\|\boldsymbol{e}_{i+\ell}\| \cdot \|\boldsymbol{e}_{i+\ell+1}\|} > C \tag{3}$$

   that is, we compute the cosine of the angle that the two error vectors form. If the vectors remain mostly parallel (i.e., that cosine is greater than C), the spatial distribution of the error has not changed much and we may continue with the current mesh, i.e.,

   - we let $\ell \leftarrow \ell + 1$
   - we *keep* the same mesh, i.e., $\mathcal{M}_m^{i+\ell} = \mathcal{M}_m^{i+\ell-1}$
   - we repeat step #3 until the Eq. 3 is *no* longer verified (i.e., $cos(\theta_\ell) \leq C$)

   This determines the maximum number of times steps ℓ for which the mesh $\mathcal{M}_m^{i+\ell}$ was valid. Then move on to step #4.

4. Compute the average error over the time span $t_i;\ t_{i+\ell}]$: $\frac{1}{\ell}\sum_{k=1}^{k=\ell} \boldsymbol{e}_{i+k}$.

   - If the error is greater than a user-prescribed tolerance, then the spatial resolution over $t_i;\ t_{i+\ell}]$ was not fine enough and we proceed with the *next* mesh adaptation (i.e., let $m \leftarrow m+1$) and, using the average error, determine the new spatial mesh $\mathcal{M}_m^{i+1}$, then return to step #2.
   - Otherwise, accept this series of time steps and return to step #1 with $i \leftarrow i + \ell$.

Fig. 1 shows the above procedure. We point out that, as the mesh adaptation proceeds (index m), a different number of valid time steps (denoted above by ℓ) may be obtained. We always stop the time marching at the smallest value of ℓ. The process we have outlined significantly reduces the bookkeeping needs and the constructions of the M^* matrix because the time marching, carried out in step #3 of the procedure, is always performed for a fixed adapted mesh.

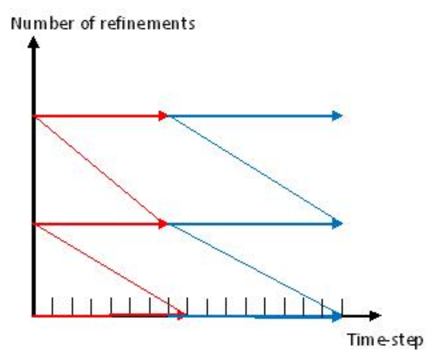

Figure 1. Spatial mesh adaptivity principle for a set of time steps

The local spatial error distribution, needed in the above procedure at each time step, is obtained with the use of *a posteriori* error estimators [9]. These error contributions are evaluated on each element K of a given mesh. These element-wise errors are easily computed using an estimator derived earlier by Kelli for Poisson's equation [10, 11]:

$$\eta_K = \sqrt{h_K}\|[\vec{\mathbf{n}} \cdot \nabla \Phi_h]\| \tag{4}$$

where h_K is the diameter of cell element K. This estimator, although obtained for Poisson's equation, has been widely used for governing equations containing Laplace operators and has been found to provide a good representation of the spatial error; see, for instance, [5].

3. RESULTS

We propose the following example. A room, of size 5 m $\times$ 4 m, contains 3 materials; the geometry is provided in Fig. 2 and the material properties are as follows: Red : $\Sigma_t = \Sigma_s = 0.01\text{cm}^{-1}$; Blue : $\Sigma_t = \Sigma_a = 0.05\text{cm}^{-1}$; Yellow : $\Sigma_t = \Sigma_s = 0.1\text{cm}^{-1}$; where the colors refer to Fig. 2. No volumetric sources are present. From $t = 0$ s until $t = 10^{-7}$ s, a photon source is applied to the left, creating a burst of particles. The photon intensity are graphed at $t = 2.10^{-9}$ s and $t = 2.10^{-7}$ s on Figs. 3 and 4; the respective meshes are provided on Figs. 5 and 6. The spatial distribution of particles has clearly evolved during that time interval.

The spatially adapted solutions have been compared to a solution using a fine uniform mesh. The CPU time comparison are given in Table I, showing a gain of 37% for the spatial adaptivity procedure.

Table I. Performance Comparison

Mesh	CPU time, sec
Uniform	667
Adapted	420

A comparison of the uniform and adapted solutions at 2×10^{-7} s is also shown in Figs. 7 and 8.

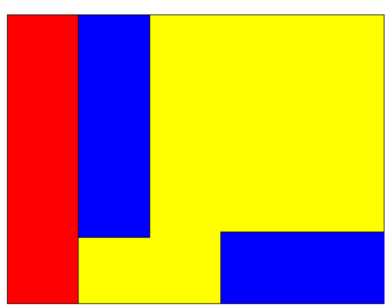

Figure 2. Problem geometry

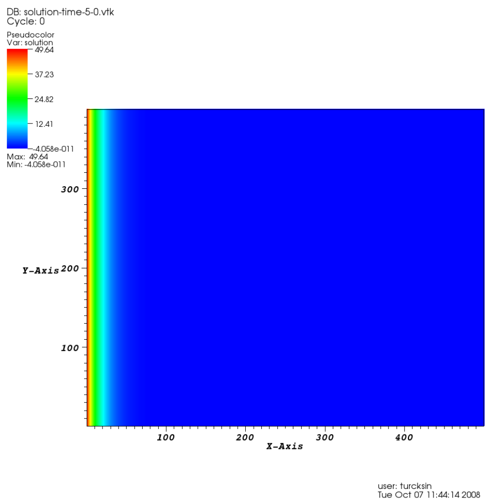

Figure 3. Intensity at 2×10^{-9} s

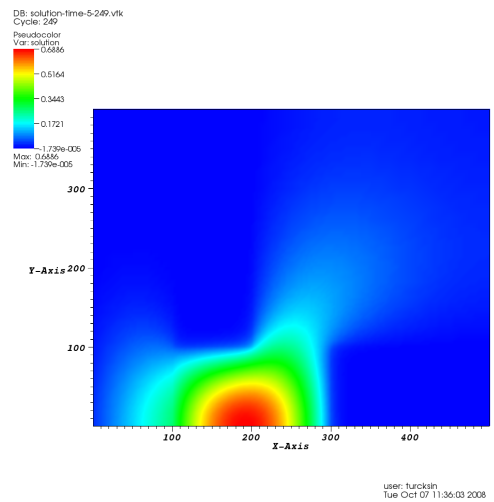

Figure 4. Intensity at 2×10^{-7} s

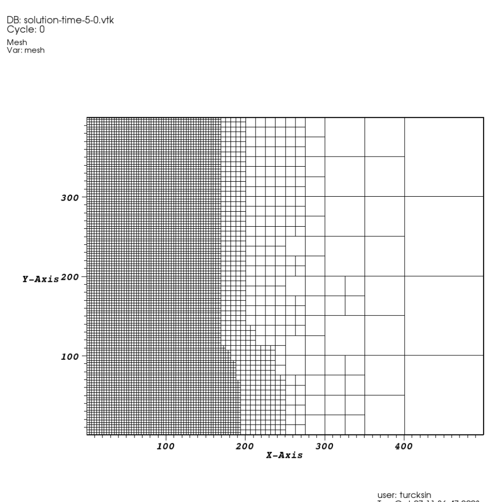

Figure 5. Mesh at 2×10^{-9} s

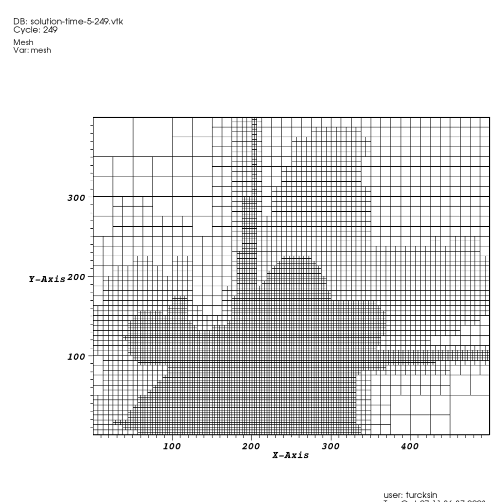

Figure 6. Mesh at 2×10^{-7} s

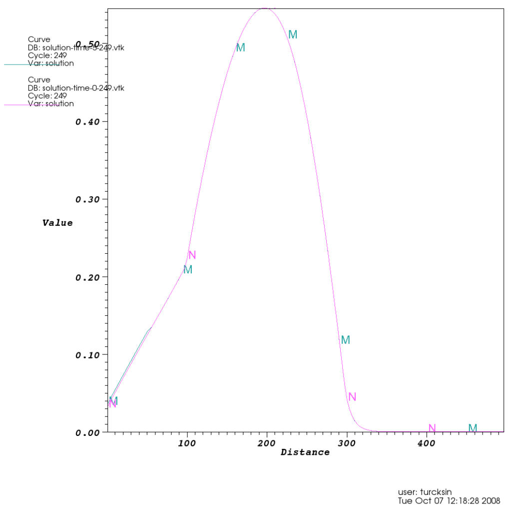

Figure 7. Comparison for $y = 50$ cm at $t = 2 \times 10^{-7}$ s

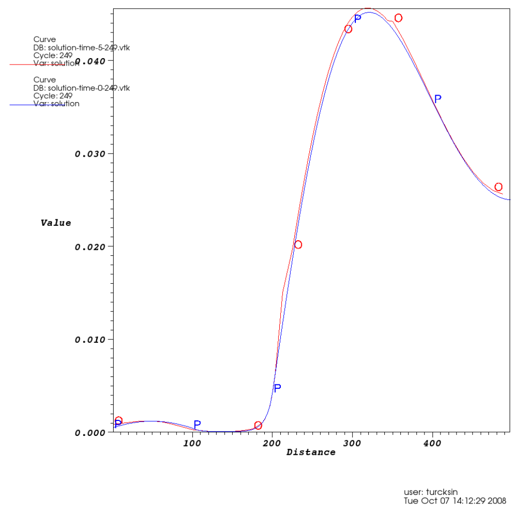

Figure 8. Comparison for $y = 300$ cm at $t = 2 \times 10^{-7}$ s

4. CONCLUSIONS

A new scheme for the efficient application of spatial adaptivity to time-dependent problems has been derived. Specifically, we avoided having recourse to several consecutive mesh adaptations per time step, but rather derived a criterion to allow the same spatial mesh to be employed for several time steps before performing a new mesh adaptation, thus reducing the computational burden while preserving the quality of the numerical solution. Therefore, the possibility of effectively solving transient problems using space-time adaptivity emerges. Even though the presentation used a simple Backward Euler temporal discretization, high-order implicit schemes can be used, opening up the possibility of combining spatial adaptivity in time (shown here) with time step control algorithms.

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