A hybrid numerical model for quickly assessing indoor contaminant transport

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Abstract

An hp-adaptive Finite Element Model (FEM) coupled with a Lagrangian Particle Transport (LPT) technique is used to simulate contaminant dispersion for emergency response assessment. The adaptive FEM accurately predicts air flow utilizing mesh enrichment along with increasing element order at locations where flow features change greatly. The use of LPT permits particles to be easily employed for predicting contaminant transport. The hybrid numerical model runs on an 18-node Beowulf PC cluster using Linux. Solutions are generally obtained quickly. The model is well suited for emergency response dispersion predictions and assessment.

Keywords: hp-adaptation, FEM, Lagrangian Particle Transport, contaminant transport, emergency response.

1 Introduction

Contaminant transport is an important environmental issue that causes serious threats to the health of the public [1]. The ability to accurately and quickly predict contaminant transport is needed to effectively assess health effects, mitigation, regulation of emissions, and effective placement of sensors. In order to design mitigation methods for control and prevention of hazardous releases, numerous numerical models that simulate air flow and contaminant transport have been developed over many years [2] - [5].

Analytical solutions for the governing equations that describe contaminant transport are generally not easy to obtain, and limited in applicability. Numerical simulation is typically the only viable means for accurately predicting contaminant transport over a wide range of conditions. In this study, an hp-
The adaptive finite element method (FEM) is coupled with a Lagrangian Particle Transport (LPT) technique to simulate indoor contaminant dispersion for emergency response assessment. A finite element scheme is used to solve the governing equations of motion. A random walk/stochastic approach is used to generate Lagrangian particles that define the contaminant dispersion trace. The use of FEM permits irregular computational domains to be easily simulated. Petrov-Galerkin weighting effectively reduces numerical dispersion associated with advection. Cost efficient computation is achieved by employing hp-adaptation technology. The LPT method permits contaminant transport traces to be quickly simulated; a general probability distribution is used for the random component of motion due to turbulent diffusion.

The hybrid numerical model converges fast, and is well suited for use in dealing with indoor emergency response dispersion predictions and assessment. Example simulations for indoor contaminant transport are presented. Efforts are underway to enable the model to link to CAD drawings of rooms and buildings to create a real-time emergency response network.

2 Finite element model

2.1 The finite element approximation

The governing equations that are used to describe indoor air flow and contaminant transport problems are generally written in the form:

Conservation of Momentum

\[ \rho \left( \frac{\partial V}{\partial t} + V \cdot \nabla V \right) = -\nabla P + \nabla \cdot (\mu \nabla V) + \rho B \]  

Species Transport

\[ \frac{\partial C_m}{\partial t} + \nabla \cdot (VC_m) = \nabla \cdot (k_n \nabla C_m) + S_{C_m} \]  

Quadrilateral and trilinear hexahedral elements are used to discretize the problem domains. The Galerkin weighted residual method has been used. The variables \( V \) and \( C_m \) can be replaced by using the trial functions:

\[ V(x,t) = \sum N_i(x) V_i(t) \]  
\[ C_m(x,t) = \sum N_i(x) C_{m_i}(t) \]

Utilizing the matrix equivalent form for the integral expressions, the governing equations can be written as:

\[ [M]\{\dot{V}\} + ([K]+[A(V)])\{V\} + C\{p\} = \{F_v\} \]  
\[ [M]\{\dot{C}\} + ([K]+[A(V)])\{C\} = \{F_{C_m}\} \]

The advection term in the momentum governing equation is weighted by Petrov-Galerkin Scheme:

\[ \int_{\Omega} \left( \frac{\partial}{\partial x_j} @ V \right) N_j \, dx = N_j \left( \frac{\partial}{\partial x_j} @ V \right) \]  

\[ W_j = N_j + \frac{\alpha h}{2|V|} \left( \frac{\partial}{\partial x_j} @ V \right) \]
\[ \alpha = \coth \beta - \frac{1}{\beta}, \quad \beta = \frac{|V| h_{e}}{2K_{e}} \]  

(8)

where \( K_{e} \) is the streamline component of diffusion tensor.

Mass lumping is used in order to obtain a fully explicit time scheme. Mass matrix is diagonalized or lumped. The inverse of the mass matrix becomes:

\[ [M]^{-1} = \frac{1}{m_{i}}. \]

### 2.2 Hp-finite element formulations

#### 2.2.1 Unstructured meshes, anisotropic and 1-irregular mesh adaptation rule for h-adaptation

Unstructured anisotropic mesh is allowed which is an efficient, directional refined mesh where refinement in one directional is needed; the 1-Irregular mesh refinement rule allows an element to be refined only if its neighbors are at the same or higher level (1-Irregular mesh), by following this rule, multiple constrained nodes (parent node themselves are constraint nodes) can be avoided.

#### 2.2.2 Minimum rule for p-adaptation

For hierarchical shape functions employed in p-adaptation, they can be categorized as: node functions, edge functions, face functions (for 3D cases) and bubble functions. The minimum rule states that the order for an edge common for two elements never exceeds orders of the neighboring middle nodes. For rectangular elements in 2D cases, both the horizontal and vertical order is considered.

#### 2.2.3 Hp constraints are employed to meet continuity requirements

As a combination of h- and p-adaptation, hp-adaptation can be either refined (unrefined) or enriched (unenriched) whenever necessary. The adaptation rules for h- and p- carry out to and combine together in hp-adaptation. Besides those, to maintain continuity of global basis function, constraints at the interface of elements supporting edge functions of different order are employed. The constraint represents a generalization of the hp-constraints is introduced by Demkowicz et al [6].

### 3 Adaptation technology

#### 3.1 Background

Adaptivity has become an active research area since the pioneering work done by Peraire et al [7], in aerodynamics for capturing shockwaves in compressible flow. Generally, two main categories existed in literature for adaptation: h-adaptation, the element sizes are varies while the orders of shape functions are constant; p-adaptation, the element sizes are constant while the order of the shape functions is increased to meet desired accuracy requirement.
Adaptive remeshing (known as r-adaptation) employs a spring analogy to redistribute the nodes in an existing mesh. In r-adaptation, no new nodes are added - the accuracy of the solution is limited by the initial number of nodes and elements. In mesh refinement, individual elements are subdivided without altering their original position. Both mesh refinement and adaptive remeshing are suitable for most fluid mechanics problems (see Nithiarasu and Zienkiewicz [8]). In this study, mesh refinement is utilized for the h-adaptation sequence.

3.2 Adaptation strategy

The combination of h- and p-adaptation produces an optimal mesh that delivers exponential convergence rates in terms of the number of degree of freedom. One of the earliest hp-adaptation strategies is known as the “three-step hp adaptive strategy” developed by Oden et al [9]. A similar strategy is followed for indoor air flow and contaminant transport simulation.

A sequence of refinement steps is employed. Three consecutive hp adaptive meshes are constructed for solving the system in order to reach a preset target error: initial mesh, the intermediate h-adaptive mesh, and the final hp adaptive mesh obtained by applying p adaptive enrichments on the intermediate mesh. The p-adaptation is carried out when the problem solution is pre-asymptotic. The procedures can be described as below:

1. Generate an initial coarse mesh
2. Compute problem solution based on current meshes
3. Compute the energy norm of the difference between the current solution and the fine mesh solution
4. if (error is less then preset error tolerance) then
   Post process the solution
   Else
      if (the computational result is not pre-asymptotic) then
         Adaptively refine mesh (h-adaptation)
         Goto step 2
      Else
         Adaptively enrich mesh (p-adaptation)
         Goto step 2
      End if
   End if

4 Lagrangian particle transport technique

4.1 Background

Most numerical methods for solving the advection-dispersion contaminant transport equation can be classified as: Eulerian Methods; Lagrangian Methods; and Mixed Eulerian-Lagrangian Methods, which are described in detail by Zheng and Bennett [10].
For Eulerian Methods, the transport equation is solved in a fixed spatial grid, it is mass conservative, and handle dispersion-dominated problems accurately and efficiently. The shortcoming is: it is susceptible to excessive numerical dispersion or artificial oscillation for advection dominated problem.

For Lagrangian Methods, a large number of moving particles are used to approximate advection and dispersion instead of solving the PDE directly; they can provide an accurate and efficient solution to advection-dominated problems. The shortcoming is: they can lead to numerical instability and computational difficulties, particularly when there is no uniform media.

Mixed Eulerian-Lagrangian Methods are conceptually attractive, as they solve the advection term with a Lagrangian approach (particle tracking) and the diffusion terms with an Eulerian approach. The shortcoming is: they do not guarantee mass conservation, and are usually not as efficient as standard Eulerian or purely Lagrangian methods.

4.2 Random walk advective and dispersive model

In this study, a Random Walk Advective and Dispersive Model (RADM) is used to predict the contaminant transport trace. This method is based on the original work of Runchal [11] and later adapted by Pepper and Carrington [12]. The concept for RADM is to solve the transport problem using a large number of particles, each of which is moved according to the equation:

$$x_t - x_0 = \int_{t_0}^{t} U(x_t, t') dt' + \int_{t_0}^{t} D(x_t, t') dw_t.$$  \hspace{1cm} (9)

where $x_0$ the initial condition and $U$ is a mean velocity vector defined over a suitable time interval and $D$ is a deterministic forcing function for the random component of motion. Eqn. (12) can be further simplified as:

$$\delta x(w, t) = \delta x_U + \delta x_D$$ \hspace{1cm} (10)

The stochastic integral may be written as:

$$\delta x_D(w, t) = \int_{t_0}^{t} n_r \sqrt{2k} dt'$$ \hspace{1cm} (11)

where $\frac{D^2}{2}$ has been assumed to be equivalent to $K$, and $n_r$ is a normally distributed random number with a mean value of zero and a standard deviation of unity.

For further simplification, eqn. (11) can be written as:

$$\delta x_D = n_r \sigma$$ \hspace{1cm} (12)

$$\sigma^2 = \int_{t_0}^{t} 2K dt'$$ \hspace{1cm} (13)

Finally the displacement equation (9) can be expressed as:

$$x_t - x_0 = \int_{t_0}^{t} U(x_t, t') dt' + n_r \left( \int_{t_0}^{t} 2K(x_t, t') dt' \right)^{1/2}$$ \hspace{1cm} (14)
For a rigorous application of the random walk method, the net particle displacement must be calculated by integration of eqn. (14). However, \( U \) and \( K \) are arbitrary functions of space and time, and it is not always possible to obtain a closed form solution to this equation. For suitably small time steps, it often proves adequate to assume that the mean velocity and the random components can be separately calculated and linearly superimposed.

In the application of RADM, \( U \) is calculated using the finite element model at the nodes of the computational domain. The random component of motion due to dispersion is calculated from a general probability distribution or correlation function.

The calculation to advance the particle in time proceeds in steps as described as follows:

\[
x_i(t + \Delta t) = x_i(t) + U_i \Delta t
\]  

(15)

The velocity components are the fictitious total velocities determined for the beginning of the time interval and initial particle positions. Every particle is advanced each time step using eqn. (15). Thus the particle traces out in time a trajectory for the pollutant material.

5 Numerical results

5.1 Problem definition

Air distribution patterns and pathways of a powder dispersing within an office are simulated using the numerical model. An office complex configuration is shown in Figure 1. There are two rooms in the office complex; one is for the secretary and the other is for the manager. Several tables are laid out in the office complex. Suppose a terrorist will put some pollutant source somewhere in the secretary room, due to the door being opened, and ventilation within the office complex, the powder spreads into the inner office. It is critically important for the inhabitants to know the contaminant transport trace accurately and quickly based on the location of the contaminant source after running our numerical model, efficient evasive actions will be taken, thus they can minimize the loss. The boundary condition and problem definition are shown in Figure 2.

Figure 1: Office complex configuration.
Two cases are examined in this study. Differences in trajectories are observed when the pollutant sources are placed at different locations inside the secretary’s room. In one case the pollutant source is placed on the top right corner of table 2, while in the other case it is placed between table 1 and table 2 in the outer secretarial room.

5.2 Computational meshes

Initial coarse computational mesh has 161 quadrilateral elements and 213 nodes, which is shown in Figure 3.

Based on the adaptation strategy presented in this paper, the final hp-adaptive mesh is obtained after two levels h-adaptation and two levels p-adaptation. Final mesh shows in Figure 4.

5.3 Results

Simulated air distribution patterns and pathways of a powder dispersing within the office complex are shown in the following series of pictures. Both the door
and the windows are open, and the contaminant powder spreads into the inner office. The sequence of pictures shows, a plan view of the flow of air and velocity vectors (Fig. 5), velocity vectors at the table height where the powder sits (Fig. 6), a 2-D plan view of the streamlines (Fig. 7).

Figure 4: hp-adapted mesh.

Figure 5: Velocity contours and vectors.

Figure 6: Table height flow patterns. Figure 7: Streamlines – plan view.
Particle dispersion pattern (using oversized particles for visualization, with red dot denotes contaminant source) shows in Figure 8 and Figure 9. The powder spreads very quickly into the inner room, and can even avoid contaminating the secretary.

![Particle dispersion pattern](image)

Case 1  Case 2

Figure 8: Particle dispersion.

As can be seen in the particle dispersion pattern, the pollutant is transported and diffused by the ventilation pattern that affects the office complex. When first responders arrive at an incident location, it is important that they be aware of the trajectory of the spreading contaminant. It is also critically important that inhabitants be aware of the contaminant pathway, and take evasive action. For example, the manager in the inner office could move to the upper left corner of his room until reached by a rescue team. Likewise, the secretary would be better off waiting at her desk instead of walking into the plume of particles.

6 Conclusions

Indoor ventilation and contaminant transport simulation using hp-adaptive Finite Element Method and Lagrangian transport technology have been presented. The hp-adaptive FEM method permits a cost efficient flow field to be constructed; while LPT permits the contaminant transport trace to be quickly simulated. The hybrid numerical model has the ability to quickly evaluate the contaminant transport status as well as provide valuable information for risk assessment associated with transport and diffusion. The fast converged numerical model is well suited for use in dealing with emergency response dispersion predictions and assessment.

References

[1] Meroney, R. N., Perspectives on air pollution aerodynamics, 10th International wind engineering conference, Copenhagen, Denmark, 1999


