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Optimal Hermite collocation applied to a one-dimensional convection-diffusion equation using an adaptive hybrid optimization algorithm

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Abstract

Purpose – The Hermite collocation method of discretization can be used to determine highly accurate solutions to the steady-state one-dimensional convection-diffusion equation (which can be used to model the transport of contaminants dissolved in groundwater). This accuracy is dependent upon sufficient refinement of the finite-element mesh as well as applying upstream or downstream weighting to the convective term through the determination of collocation locations which meet specified constraints. Owing to an increase in computational intensity of the application of the method of collocation associated with increases in the mesh refinement, minimal mesh refinement is sought. Very often this optimization problem is the one where the feasible region is not connected and as such requires a specialized optimization search technique. This paper aims to focus on this method.

Design/methodology/approach – An original hybrid method that utilizes a specialized adaptive genetic algorithm followed by a hill-climbing approach is used to search for the optimal mesh refinement for a number of models differentiated by their velocity fields. The adaptive genetic algorithm is used to determine a mesh refinement that is close to a locally optimal mesh refinement. Following the adaptive genetic algorithm, a hill-climbing approach is used to determine a local optimal feasible mesh refinement.

Findings – In all cases the optimal mesh refinements determined with this hybrid method are equally optimal to, or a significant improvement over, mesh refinements determined through direct search methods.

Research limitations – Further extensions of this work could include the application of the mesh refinement technique presented in this paper to non-steady-state problems with time-dependent coefficients with multi-dimensional velocity fields.

Originality/value – The present work applies an original hybrid optimization technique to obtain highly accurate solutions using the method of Hermite collocation with minimal mesh refinement.

Keywords Meshes, Optimization techniques, Programming and algorithm theory

Paper type Research paper

1. Introduction

The method of collocation, while simple to implement, has not traditionally been the preferred finite-element approach taken when determining a numerical solution to groundwater flow and transport models. Advances in this method were made early in the development of finite-element theory when it was found that for certain differential equations, the collocation locations that minimize local discretization error occur at the points of Gaussian quadrature for each element in the finite-element mesh (Prenter,

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1975; de Boor, 2001). While this advancement found that the approximate solution at the collocation locations minimized local discretization error, it did not solve the difficulties inherent in oscillatory artifacts associated with the application of collocation to solve for transport migration in a convection driven flow field.

Improvements in the method of collocation applied to the convection-diffusion equation occurred in the mid-1980s. Upstream collocation on Hermite cubics as compared to orthogonal collocation with respect to effective diffusion was found to replace one type of numerical artifact (non-physical oscillations) for a more desirable one, namely numerical diffusion in the solution to the convection-diffusion equation (Dougherty and Pinder, 1982). Soon after this, Allen found that by using upstream weighting on the convective term, i.e. assigning a different collocation location for different terms in the convection-diffusion finite-element approximation, oscillations could be reduced in the numerical approximation (Allen, 1983). These results were taken one step further when it was shown that by careful refinement of the finite-element mesh, the approximation could be substantially improved for accuracy (Brill, 2004).

Determining the solution to partial differential equations using collocation methods reduces to solving linear systems that are in general non-symmetric and non-diagonally dominant. For this reason one focus on improving the efficiency of collocation methods has been to develop approaches that simplify the associated linear system. One such technique involved block iterative methods for the collocation equations of elliptic PDEs defined on a rectangular domain and subject to uncoupled mixed boundary conditions (Lai *et al.*, 1994). More recent advances with this focus have involved techniques that reduce the number of unknowns associated with each node in the discretization. One such method uses polynomials to approximate the first-order derivatives of the solution to the flow and transport equations over a construct about each node in the discretization (Fedele *et al.*, 2004). Another method that is structured on multiquadrics radial basis functions effectively changes the traditional global collocation approach to one that is made locally over a set of overlapping domains of influence (Vertnik and Sarler, 2006). In this approach, small linear systems with dimension equal to the number of nodes in each domain must be solved. This method and further advances in this methodology have been illustrated both on the convection problem in porous media as well as in more complex systems (Kosec and Sarler, 2008; Vertnik and Sarler, 2006). Further studies using the radial basis functions include the double boundary collocation Hermitian approach for the solution of steady-state convection-diffusion problems (LaRocca and Power, 2007). In this approach, at the boundary collocation points the boundary condition and the governing partial differential equation are required to be satisfied simultaneously, resulting in higher precision results, especially for prediction of the fluxes at the boundaries.

While finding techniques that decrease the computational intensity associated with collocation techniques is one focus of interest, others involved in the study of the methods of collocation have focused on the accuracy and precision of the resultant solutions. A coordinate transform approach that couples solutions using a finite difference approach to a method that utilizes Hermite collocation is developed to address one-dimensional differential problems with steep solutions (Lang and Sloan, 2002). Recent advances in finding accurate solutions for three-dimensional boundary value problems using the method of collocation have involved applying genetic algorithms to determine optimal arrangements of collocation points (Zieniuk *et al.*, 2005).

In general numerical methods used for solving differential equations improve in accuracy with mesh refinement. The computational intensity of numerical methods is almost always directly related to the discretization of the solution space, i.e. the mesh complexity. Useful numerical solvers are computationally intensive and require the use of computer technology to implement. While computer technology is capable of performing numerical tasks, the technology is limited and hence, it is advantageous to the modeler to minimize the required computations for a given algorithm. The mesh refinement exercise for Brill's optimized finite-element application is one such example where it is advantageous to obtain a mesh refinement that contains the smallest number of nodes such that the constraints placed on the system are satisfied.

This paper presents an adaptive genetic algorithm followed by a hill-climbing algorithm that is used to determine an optimal refinement of the steady-state finite-element mesh used to approximate the solution to the convection-diffusion equation in one dimension. This hybrid optimization algorithm determines a new finite-element mesh for the proposed system as well as the upstream or downstream collocation locations for the convective term. In doing so, the method of collocation in conjunction with the determined mesh refinement can be used to efficiently determine an accurate solution to the convection-diffusion equation.

This optimization algorithm is one that can be used for any discretization problem where the constraints of the discretization have been determined for highly accurate solutions. The application of this optimization algorithm to the one-dimensional steady-state convection-diffusion problem where Hermite collocation is applied is one such example where the necessary constraint calculations have been made.

2. Collocation and constraints

The convection-diffusion equation consists of a differential equation with two terms, one that describes transport due to convection and another that describes transport due to diffusion:

$$-D\frac{d^2u}{dx^2} + v\frac{du}{dx} = 0. \tag{1}$$

The equation is defined over the interval (0, 1) with given Dirichlet boundary conditions:

$$u(0) = 1 \tag{2}$$

$$u(1) = 0 \tag{3}$$

The parameter D describes the diffusion, which is assumed to be constant over the entire region considered. The parameter v is the velocity of the groundwater and may vary over the entire region; however, it is assumed to be a constant value on each element in the finite-element mesh. The function $u(x)$ is the concentration of the contaminant in the groundwater and is the function to be approximated using the method of collocation. The values of u_L and u_R are constant concentration values at the boundaries of the domain.

It should be noted that the steady-state one-dimensional convection-diffusion equation as is presented may not satisfy mass conservation, and this is a limitation of this model. The application of optimal Hermite collocation to this one-dimensional steady-state model, however, provides the approach that should be taken to solve more complicated problems, such as those where mass conservation is satisfied. As such, the methods presented in this paper can be generalized to non-steady-state, time-dependent problems in higher dimensions.

The method of collocation is one that falls under the category of the "method of weighted residuals" in the field of finite-element analysis. In finite-element analysis, the weighted sum of specified base functions over each element is used to approximate the solution to a differential equation. To solve the one-dimensional convection-diffusion equation using the method of collocation two points of collocation must be specified for each element in the discretization. These points of collocation are fixed for each element prior to the application of the method of collocation and affect the accuracy of the determined approximation to the solution. As such the collocation points are decision variables in the search for an optimally accurate approximation to the convection-diffusion equation using the method of collocation.

For example the true solution of a one-dimensional problem, $u(x)$, is approximated by a linear combination of $n+1$ predetermined basis functions, $\hat{u}_i$, where n is the number of elements in the finite-element mesh and so $n+1$ is equal to the number of nodes in the mesh:

$$\hat{u}(x) = \sum_{i=1}^{n} w_i \tilde{u}_i(x). \tag{4}$$

In the method of weighted residuals, the value of the weights, w_i, is determined by setting the weighted errors (or weighted residuals) of this approximation over the domain of the problem equal to zero. This amounts to finding those w_i values such that the residual times a weighting function defined locally to each element is equal to zero. The residual is the integral of the differential operator applied to the approximation to the solution.

When the Dirac-delta function is used as the weighting function for the method of weighted residuals, this focuses the residual to the point where the Dirac-delta function is not equal to zero. This point is called the collocation location, x_k. The method of collocation is then just a finite-element method that utilizes the method of weighted residuals where the weights are defined to be the Dirac-delta functions, $\delta(x)$. The integral that is satisfied is

$$\int_B R(\hat{u}(x))\delta(x - x_k)dx = 0 \quad \text{for } k = 1..m = 2n - 2. \tag{5}$$

The parameter B represents the boundary of the region over which the differential equation is defined and R is the residual function defined as

$$R(\hat{u}(x)) = -D\frac{d^2\hat{u}}{dx^2} + v\frac{d\hat{u}}{dx} \tag{6}$$

Clearly $R(\hat{u}(x)) = 0$ for each collocation location x_k.

When using the method of collocation to approximate the solution to the convection-diffusion equation in one dimension, it has been shown that upstream weighting applied to the convective term can minimize numerical artifacts associated with the method of collocation (Allen, 1983). Through refinement of the finite-element mesh in a precise manner, along with upstream or downstream weighting, the numerical artifacts associated with the method of collocation can be eliminated and the results of approximation are highly accurate (Brill, 2004).

Brill has successfully determined the required mathematical relationships between the locations of the nodes and the collocation locations for the convective and diffusive terms for each element so that the method of collocation results in highly accurate numerical approximations to the true solution of our convection-diffusion equation (Brill, 2004). The parameters of these relationships include:

- an initial number of elements for the model, p
- the velocity of the groundwater over each element, $v_1, v_2, \ldots, v_p$
- the diffusivity for the contaminant, D, which is constant over the entire model.

The refinement of the original mesh prescribed will be such that the ith element will be divided into m_i equally spaced elements and the collocation locations. The value of ζ_i is defined locally over element i and as such only assumes values between $-1/2 + 1/\sqrt{12}$ and $1/2 - 1/\sqrt{12}$. In this work, however, ζ_i, will fall within bounds set in Brill's 2004 paper.

To search for the minimum mesh refinement, begin by determining the largest index, i, associated with the element assigned the highest velocity value for the groundwater model. This index is called the kth index and so $v_k \geq v_i$ for all $i \neq k$. It is over this kth element that there is a single equation that relates the element's refinement, m_k, to the collocation locations over this element, $\pm 1/\sqrt{12} - \zeta_k$ (see the Appendix) (Brill, 2004). Given a fixed m_k, ζ_k is determined to be the root of a quadratic equation.

All other ζ_i (where $i \neq k$) values can be determined from fixed m_k and m_i values through the use of equations derived by Brill and presented in the Appendix of this paper. These equations relate consecutive elements in such a way that the unknown ζ_i values can be determined as long as m_i is known as well as either (1) ζ_{i-1} and m_{i-1} are known or (2) ζ_{i+1} and m_{i+1} are known. In both cases, ζ_i is determined to be the root of a polynomial of potentially high degree. Numerical methods must be used to determine such a root. It is sufficient that only one root of this polynomial be within the bounds set by Brill. This root is the assigned ζ_i value.

To summarize, once an m_k value is found such that ζ_k falls within the assigned bounds set for all ζ_i values, one can fix all other m_i values where $i \neq k$ and determine the associated ζ_i values. The goal is to find values of m_i such that (1) $\sum_{i=1}^{p} m_i$ is minimized and (2) ζ_i satisfy their given constraints.

3. Optimization problem

The convection-diffusion equation can be solved with very high accuracy using the method of collocation provided certain relationships exist between the location of the nodes of the finite-element mesh and the collocation location assigned to the convective term in the convection-diffusion equation (Brill, 2004). Obtaining the relationships necessary for the application of collocation with highly accurate solutions often requires refinement of a crude finite-element mesh that may have been defined with the intent to capture physical distinctions within the model, such as spatially variable changes in parameter values. Because computational intensity involved in the application of the method of collocation is related to the number of elements prescribed in the model, it is advantageous to determine a minimal mesh refinement that optimizes the numerical accuracy of the approximating solution.

The optimization problem for maximum accuracy and minimum computational intensity associated with finding the solution to the convection-diffusion equation using the method of collocation is derived in the following manner. The objective function is the sum of the number of elements in the finite-element mesh. In order to minimize the computational intensity associated with using the method of collocation, the sum of the number of elements is minimized.

The constraints of this optimization problem consist of conditions that must be satisfied between the points of upstream/downstream weighting, ζ_i, and the mesh refinement, m_i, for each element i. These conditions were derived by equating the solution to the convection-diffusion equation determined through analytic methods to the analytical solutions of upstream Hermite collocation. By equating these solutions at each node of the finite-element mesh, Brill showed that maximum accuracy in the application of the method of collocation is obtained for this problem. Additional constraints placed upon this optimization problem include that of restricting the upstream weighting to the support of the basis functions used in Hermite collocation, 1/2, plus or minus $1/\sqrt{12}$, which are the points of Gaussian quadrature. The number of elements must be within the set of positive integer values and the upstream weight for each element is within the set of complex values. The initial finite-element mesh consists of p elements.

The formulation of the optimization problem is given by

minimize:

$$\sum_{i=1}^{p} m_i \tag{7}$$

subject to:

$$G(\zeta_k, m_k) = 0 \tag{8}$$

$$F_i(\zeta_i(m_i, \zeta_{i+1}, m_{i+1})) = 0 \tag{9}$$

$$H_i(\zeta_i(m_i, \zeta_{i-1}, m_{i-1})) = 0 \tag{10}$$

$$|\zeta_i| \leq \frac{1}{2} - \frac{1}{\sqrt{12}} \tag{11}$$

$$m_i \in \mathbf{Z}^+ \text{ and } \zeta_i \in \mathbf{R} \quad \forall i = 1..p \tag{12}$$

where m_i is the number of new elements, i.e. the mesh refinement in element i, $\mathbf{Z}^+$ denotes the set of positive integers and $\mathbf{R}$ denotes the set of real numbers. If $m_i = 1$, then no mesh refinement occurs. The value k is a fixed integer that is equal to the largest index of the element with the largest value of velocity in the physical model. The value p is the number of elements in the original physical model. The value of ζ_i is the amount of upstream weighting, when ζ_i is determined to be greater than zero, or downstream weighting, when ζ_i is determined to be less than zero, applied to the convective term, and hence is related to the collocation location for the convective term over element i. The functions G, F and H refer to the relationships prescribed by Brill in order to obtain maximum accuracy in the application of the method of collocation for this problem. These functions are described in detail in the Appendix.

The optimization problem is to find the vector $\mathbf{m} = (m_1, m_2, \ldots, m_p)$ such that the sum of the components of $\mathbf{m}$ is minimized while the ζ_i values all adhere to the prescribed relationships given by the functions G, F and H and that the ζ_i values all fall within the required upper and lower bounds. The boundaries placed upon the ζ_i values vary non-linearly as a function of $\mathbf{m}$, so while the objective function for this problem is linear, the nature of the non-linearity of the constraints results in a feasible region that is non-convex.

Through a direct search method Brill has determined discretizations that result in highly accurate approximations (Brill, 2004). This work, however, was conducted on a problem where there were initially only four initial elements in the finite-element mesh. As the number of initial elements considered in this problem increases, the dimensionality of the problem increases and a direct search method is not an efficient search technique for determining a discretization that results in highly accurate solutions.

4. Optimization solver: hybrid search technique

The constrained optimization problem is transformed into an unconstrained optimization problem so that global optimization techniques can be employed. Violations of those constraints that pertain to the ζ_i values are permitted, however, when this occurs, a penalty term is added to the value of the objective function.

If it is found that, given a fixed **m**, at least one of the polynomials G, F and H does not have a real root, then a violation value is determined for that **m**. Examining the complex roots for each polynomial with the smallest magnitude, ζ_i, the violation is determined to be the sum of the Euclidian distances from the violating ζ_i values to the closest boundary value placed upon all ζ_i values, namely $1/2 - 1/\sqrt{12}$ or $-1/2 + 1/\sqrt{12}$. Once the sum of the violations has been determined, this value is multiplied by a penalty weight, ϕ, then added to the sum of the m_i values to obtain the value of the transformed objective function. This modification of the optimization problem is expressed as
Objective:

$$\min \sum_{i=1}^{p} (m_i + \phi * \max(0, \xi_i)) \tag{13}$$

Subject to:

$$G(\zeta_k, m_k) = 0 \tag{14}$$

$$F_i(\zeta_i(m_i, \zeta_{i+1}, m_{i+1})) = 0 \tag{15}$$

$$H_i(\zeta_i(m_i, \zeta_{i-1}, m_{i-1})) = 0 \tag{16}$$

$$m_i \in \mathbf{Z}^+ \text{ and } \zeta_i \in \mathbf{C} \quad \forall i = 1..p \tag{17}$$

where ξ_i is given by

$$\xi_i = \begin{cases} 0, & \text{if} \zeta_i \in \mathbf{R} \text{ and } |\zeta_i| \leq \frac{1}{2} - \frac{1}{\sqrt{12}} \\ \sqrt{\left(\mathrm{Re}(\zeta_i) - \left(\frac{1}{2} - \frac{1}{\sqrt{12}}\right)\right)^2 + (\mathrm{Im}(\zeta_i))^2}, & \text{if} \zeta_i \in \mathbf{C}, \zeta_i \notin \mathbf{R} \text{ and } \mathrm{Re}(\zeta_i) \geq 0 \\ \sqrt{\left(\mathrm{Re}(\zeta_i) - \left(-\frac{1}{2} + \frac{1}{\sqrt{12}}\right)\right)^2 + (\mathrm{Im}(\zeta_i))^2}, & \text{if} \zeta_i \in \mathbf{C}, \zeta_i \notin \mathbf{R} \text{ and } \mathrm{Re}(\zeta_i) < 0 \end{cases}$$

and **C** denotes the set of complex numbers.

While it may seem that the objective function is now a function of continuous variables, namely ζ_i, this is not the case. Recall that the ζ_i values are dependent upon the integer values m_i. This optimization problem remains of the integer type; however, the transformation performed has rendered the objective function non-linear.

The method used to solve this optimization problem is a hybrid method that consists of cycling through two search phases: an adaptive genetic algorithm (AGA) and a local gradient search (GS) algorithm. The objective of the first phase, the AGA phase, is to obtain a solution that is within close proximity of a local optimal solution. In the second phase, the GS phase, a local search is conducted to obtain the local optimal solution in the region determined. Parameters that define the search space of the genetic algorithm within the AGA phase are updated at the start of each cycle of the search. By changing these parameters the optimization algorithm is able to improve its efficiency in determining feasible regions that are not connected where improved locally optimal solutions may exist. For the problem considered in this paper two regions are not connected if the minimum distance between these regions is greater than one. A connected region is one where the distance between any point in the region and its nearest neighbor is not greater than one. The search algorithm terminates when the solutions to successive cycles does not result in an improved locally optimal solution. Because of the discrete nature of this optimization problem and the nonlinearity in this problem, there are no current optimization techniques developed that ensure that the determined local solution is the global solution; however, this does not preclude one from using the available techniques to determine a reasonable solution.

4.1 Adaptive genetic algorithm

Each cycle of the hybrid optimization solver begins with the application of an AGA. To begin the AGA (Holland, 1992) value encoding is employed so that a parent population of size N of the $\mathbf{m}$ vectors is created by randomly selecting positive integer values for each m_i variable within some prescribed range of values. In the first cycle of this solver, the upper bound is based upon preliminary analysis of the problem to determine a value that, when setting all elements of the $\mathbf{m}$ vector equal to it, will result in a feasible solution. In subsequent cycles of this solver, the upper bound is set equal to the sum of elements of the most recently determined local optimal solution, $\sum_i^n m_i^*$. The lower bound, for all m_i where $i \neq k$ is 1. And the lower bound for m_k is set equal to the minimum value of m_k such that $|\zeta_k| \leq 1/2 - 1/\sqrt{12}$. It is the adaptive nature of the upper bound of the genetic algorithm that increases the efficiency of this algorithm for determining locally optimal solutions in feasible regions that are not connected.

Once a parent population has been determined at the start of each cycle a fitness value is assigned to each member of the population. This fitness value is defined to be the sum of the m_i values plus a penalty term associated with any violations of the ζ_i constraints (Equation 11).

After a parent population has been determined and a fitness value has been assigned to each member of the parent population, a new population is derived from a subset of the parent population. This new population, referred to as the child population or the next generation, will contain the same number of members as the parent population. The derivation of the child population entails a number of processes.

In determining the child population from the parent population, elitism is employed, i.e. some members of the parent population that have the best fitness values become members of the child population.

Members of the child population not obtained through elitism are derived from a subset of the parent population with the highest fitness values (including those members that were involved in elitism). These members of the child population are created through recombination of the given set of parents. This recombination involves crossover and mutation.

In one single point crossover event, two parents, $\mathbf{m^{P1}}$ and $\mathbf{m^{P2}}$, are randomly selected from that subset of the parent population that meets the fitness criteria set by the modeler for recombination. In crossover, a new vector of p integers, the child, $\mathbf{m^{C}}$, is created by taking a combination of the two parent strings in the following manner. The first s elements of $\mathbf{m^{C}}$ are equal to the first s elements of $\mathbf{m^{P1}}$, while the remaining $p - s$ elements of $\mathbf{m^{C}}$ are equal to the final $p - s$ elements of $\mathbf{m^{P2}}$ (Table I).

There is only one crossover location, s, in this algorithm; however, this crossover location is randomly selected for each crossover event. Random crossover events are conducted until the child population has as many members as the parent population.

Crossover events and elitism do not introduce new integer values into the population. To introduce new integer values into each string of m_i's in each population, random integer values are changed or mutated after each crossover event (Table I). The number of integers that undergo mutation is determined through a mutation rate set by the modeler. Members of the child population that have been determined through elitism do not undergo mutation.

The child population generated from the original parent population is referred to as the first generation. After this first child population is obtained, this population acts as a parent population for a new generation or new child population. The nth generation is used to obtain the $(n + 1)$st generation, whose fitness values for the best fit members are equal to, or surpass the fitness values of the generation from which they were derived.

The genetic algorithm ends when a maximum number of generations has been derived. Because of the random nature of the genetic algorithm, no assurance can be made that the algorithm results in a global optimal solution. Only an exhaustive search of $\mathbf{m}$ vectors with incrementally larger magnitudes can make this assurance. As the number of elements considered in the physical model increases, however, an exhaustive search is not feasible.

4.2 Local search

Preliminary results have indicated that the nature of this optimization problem is such that the optimal values of $m_1, m_2, \ldots, m_p$ may vary by orders of magnitude (Brill, 2004). Due to this variation, convergence to a local optimal solution using an AGA is inhibited. At later stages of the AGA, the populations approach uniformity, i.e. the members of the population are very similar and crossover events are not effective in generating members of a child population with improved fitness values. Improvements in fitness become reliant upon mutation. Values of m_i that are relatively low are closer

Table I. Creation of a member of a child population of length $p = 15$ from a single crossover event where the random crossover location is at $s = 5$

	Integer string of length $p = 15$														
Parent 1	**3**	**8**	**4**	**14**	**5**	*8*	*2*	*3*	*1*	*6*	*4*	*9*	*1*	*2*	*3*
Parent 2	*4*	*9*	*5*	*7*	*2*	**4**	**9**	**2**	**26**	**5**	**7**	**4**	**8**	**17**	**2**
Child	**3**	**8**	**4**	**14**	**5**	**4**	**9**	**2**	**26**	**5**	**7**	**4**	**8**	**17**	**2**
Mutated child	**3**	**8**	*21*	**1**	**5**	**4**	**9**	*7*	**26**	**5**	**7**	*1*	**8**	**3**	**2**

Note: The child is then mutated with a mutation rate 20 percent, which affects three elements of the child vector to their optimal value than m_i values which are large, and hence, the most beneficial mutation events are dependent upon (1) the mutation rate, which is typically set to be a low value, (2) the mutation direction being one that results in an improvement of the fitness of **m** and (3) the likelihood of the mutation occurring at an m_i value that leads to substantial improvement of the fitness of **m**. The conditions for beneficial mutation occurring at later stages of this AGA are not frequent, and convergence to a local optimal is slow. For this reason, a local search algorithm is developed for this problem.

While the AGA is not an efficient method for determining a local optimal **m** for this problem, the AGA is very effective at determining a region where a locally optimal solution exists. After the AGA has determined a region where a locally optimal solution exists, the newly developed local search is used to determine the true local optimal.

The local search that has been developed is specifically designed for this integer problem that contains scaling issues and known trajectories for improvement in the feasible region. The local search determines the fitness values of a number of **m** vectors within the vicinity of the solution determined with the AGA. This set will contain at most p neighboring **m** vectors determined in the following manner. First a step size that is directly related to the size of m_i is determined for each i direction. Each member of the neighboring set is the same as the **m** determined through the GA except the m_jth element. The m_jth element is set equal to m_j from the solution to the AGA minus the jth step size. If this step results in a vector where either the fitness value has not improved or the original constraints for the optimization problem are violated then the magnitude of the step size is reduced to the greatest integer closest to the original magnitude reduced by one-half. The search for a better-fit-feasible neighbor that varies in the jth element is implemented with the reduced step size. Reduction of the step size continues until a neighboring vector is determined to have an improvement in fitness and zero penalty. If the jth step size is determined through the reduction process to be less than one, this implies that the solution to the AGA cannot be improved in the jth direction, and no neighboring vector is included in the neighboring set (Table II).

Once the neighboring set has been determined, the vectors within the set are ranked according to their fitness values. The best fit solution in the neighboring set is then determined. The region of this new best solution is examined in the local search, which continues until the neighboring set contains no vectors. The last best fit solution is the locally optimal solution in the region of the solution determined through the AGA.

5. Example problems

The search for an optimal mesh refinement for the application of the method of collocation to solve our convection-diffusion equation is applied to 12 one-dimensional problems with (initially) four equally spaced nodes. These models are broken up into two groups that differ in the values of the diffusivity constants. The first group has a

m =	2	42	3	1
Step size	1	5	1	1
Neighbors				
Neighbor (1)	1	42	3	1
Neighbor (2)	2	37	3	1
Neighbor (3)	2	42	2	1
Neighbor (4)		none		

Table II. An example of a neighboring set of **m** where $p = 4$

diffusivity constant of 5, while the second group has a diffusivity constant of 1. The six subgroups differ in the velocity values assigned to each node. These 12 example problems along with the optimal mesh refinement values are listed in Tables III and IV. Additionally, four one-dimensional problems with eight equally spaced nodes and where $D = 1$ are examined (Table V).

The penalty weight for the problem where $D = 5$ is $\phi = 100$ and where $D = 1$ is $\phi = 200$. Violations in the constraints will be multiplied by this value and added to the objective function so that this optimization problem can be viewed as an unconstrained optimization problem.

The parameters of the genetic algorithm are listed in Table VI. The mutation rate is 20 percent for this problem, which is a very high value for most genetic algorithms. In this problem the string of integers to be optimized contains either four or eight elements, and so a mutation rate of less than 25 percent is sufficiently small for optimization.

6. Results

Optimal mesh refinements determined with the hybrid optimization algorithm are listed in Tables III-V. The hybrid method was run for each example 100 times, each with a different randomly generated initial parent population. In all instances where a direct search method has been previously examined for the problem the solutions

Table III. Values of parameters in the computational examples. $D = 5$

Example number	D	j	v_j	Direct search m_j	Hybrid search m_j	Solution frequency	Hybrid search ζ_j	Hybrid maximum error
1	5	1	100.0	41	24	100%	-1.259×10^{-5}	2.187×10^{-14}
		2	0.1	8	1		2.100×10^{-1}	
		3	10.0	8	1		-8.473×10^{-4}	
		4	1.0	8	1		1.324×10^{-1}	
2	5	1	0.1	1	1	100%	-2.097×10^{-1}	6.661×10^{-16}
		2	100.0	24	24		-1.259×10^{-5}	
		3	10.0	1	1		-8.085×10^{-4}	
		4	1.0	1	1		1.288×10^{-1}	
3	5	1	10.0	1	1	100%	6.149×10^{-4}	6.772×10^{-15}
		2	0.1	1	1		-2.097×10^{-1}	
		3	100.0	24	24		-1.259×10^{-5}	
		4	1.0	1	1		2.074×10^{-3}	
4	5	1	0.1	2	1	100%	-3.886×10^{-2}	1.669×10^{-8}
		2	1.0	2	1		3.781×10^{-4}	
		3	10.0	2	2		-1.090×10^{-4}	
		4	100.0	17	17		-3.552×10^{-5}	
5	5	1	0.1	1	1[a]	72%	-2.089×10^{-1}	2.153×10^{-8}
		2	100.0	43	42		2.514×10^{-6}	
		3	0.1	1	1		-2.235×10^{-2}	
		4	100.0	41	42		-2.345×10^{-6}	
6	5	1	100.0	9	1	100%	1.908×10^{-2}	2.142×10^{-14}
		2	0.1	9	1		-2.097×10^{-1}	
		3	100.0	42	24		-1.259×10^{-5}	
		4	0.1	9	1		2.100×10^{-1}	

Note: [a]Multiple solutions of equal value are determined. See the text for these solutions

Example number	D	j	v_j	Direct search m_j	Hybrid search m_j	Solution frequency	Hybrid search ζ_j	Hybrid maximum error
7	1	1	100.0	108	54	100%	-1.396×10^{-4}	1.121×10^{-4}
		2	0.1	16	1		2.076×10^{-1}	
		3	10.0	16	2		-4.804×10^{-3}	
		4	1.0	16	1		1.819×10^{-1}	
8	1	1	0.1	1	1	100%	-2.061×10^{-1}	1.142×10^{-4}
		2	100.0	97	54		-1.396×10^{-4}	
		3	10.0	11	2		-4.743×10^{-3}	
		4	1.0	1	1		1.798×10^{-1}	
9	1	1	10.0	1	1	100%	8.567×10^{-3}	1.776×10^{-15}
		2	0.1	1	1		-2.061×10^{-1}	
		3	100.0	54	54		-1.396×10^{-4}	
		4	1.0	1	1		1.798×10^{-3}	
10	1	1	0.1	1	1	91%	-1.729×10^{-1}	5.3291×10^{-15}
		2	1.0	1	1		1.476×10^{-3}	
		3	10.0	4	4		-5.855×10^{-4}	
		4	100.0	36	36		-4.790×10^{-4}	
11	1	1	0.1	1	1[a]	32%	-2.108^{-1}	3.962×10^{-8}
		2	100.0	145	139		6.887×10^{-6}	
		3	0.1	1	1		-3.949×10^{-3}	
		4	100.0	139	145		-7.131×10^{-6}	
12	1	1	100.0	18	1	100%	-4.000×10^{-2}	Code failed to produce a solution
		2	0.1	18	1		-2.061×10^{-1}	
		3	100.0	111	54		-1.396×10^{-4}	
		4	0.1	18	1		2.076×10^{-1}	

Note: [a]Multiple solutions of equal value are determined. See the text for these solutions

Table IV. Values of parameters in the computational examples. D=1

determined with the hybrid algorithm are equal to or an improvement over previous results (Brill, 2004).

The value of D is set equal to 5 in Examples 1 through 6. This differs from the value of D set in Examples 7 through 12, which is 1. Other than this difference for Examples 1 through 12 Example 1 is the same as Example 7, Example 2 is the same as Example 8, etc. The value of D is set equal to 1 in Examples 13 through 16, and the velocity fields are variations of Example 10 and Example 7.

The results from Examples 1 and 6 are a vast improvement over the direct search method. One phase cycle of the hybrid algorithm inclusive of the AGA and the GS was utilized to determine these solutions. The solution for Example 1 is $\mathbf{m} = (24, 1, 1, 1)$ (Figure 1) and the solution for Example 6 is $\mathbf{m} = (1, 1, 24, 1)$. In both of these examples, the solutions were determined in 100 percent of the runs. The numerical solution is equal to the true solution at the collocation locations; however, it is only an approximation to the solution at the nodes. The maximum error is calculated to be the maximum difference between the numerical approximation and the true solution at all of the nodes within the finite-element mesh. The maximum errors of the numerical solutions determined with these discretizations are 2.187×10^{-14} and 2.142×10^{-14}, respectively.

The direct search results for Examples 2 and 3 are identical to the results determined using the hybrid algorithm in 100 percent of the runs. The maximum errors are 6.661×10^{-16} and 6.772×10^{-15}, respectively. One phase cycle of the hybrid algorithm was utilized to determine these solutions.

Table V.
Values of parameters in the computational examples. $D = 1$

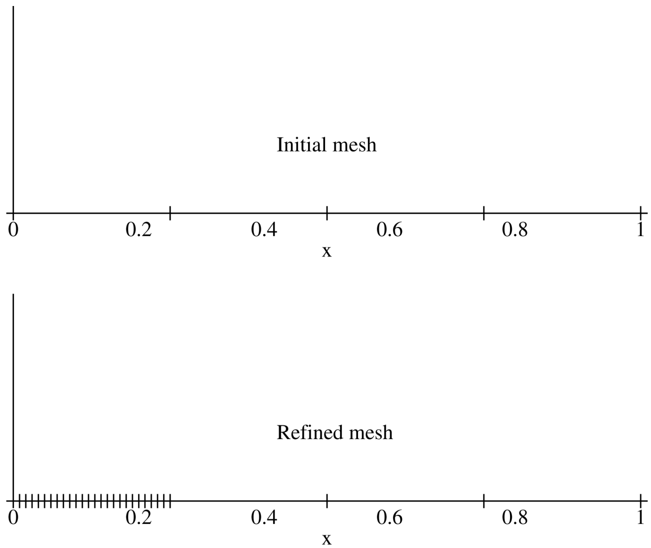
Example number	D	j	v_j	Hybrid search m_j	Solution frequency	Hybrid search ζ_j	Hybrid Maximum error
13	1	1	0.1	1[a]	6%	-2.076×10^{-1}	5.854×10^{-12}
		2	1.0	1		1.993×10^{-3}	
		3	10.0	4		-1.629×10^{-4}	
		4	100.0	59		-1.246×10^{-6}	
		5	0.1	1		3.374×10^{-3}	
		6	1.0	2		-7.161×10^{-5}	
		7	10.0	7		-1.627×10^{-5}	
		8	100.0	63		-1.087×10^{-5}	
14	1	1	0.1	1	100%	1.472×10^{-1}	1.195×10^{-12}
		2	0.1	1		-1.458×10^{-1}	
		3	1.0	1		1.384×10^{-3}	
		4	1.0	1		-1.333×10^{-3}	
		5	10.0	4		-5.459×10^{-5}	
		6	10.0	5		3.002×10^{-5}	
		7	100.0	44		-3.509×10^{-5}	
		8	100.0	43		-3.429×10^{-5}	
15	1	1	100.0	1[a]	70%	3.257×10^{-2}	7.812×10^{-1}
		2	0.1	1		-1.991×10^{-1}	
		3	10.0	7		9.757×10^{-5}	
		4	1.0	1		-1.044×10^{-3}	
		5	100.0	45		-2.991×10^{-5}	
		6	0.1	1		1.063×10^{-1}	
		7	10.0	2		-8.272×10^{-4}	
		8	1.0	1		4.635×10^{-2}	
16	1	1	100.0	1	100%	3.256×10^{-2}	9.436×10^{-1}
		2	100.0	38		-4.976×10^{-5}	
		3	0.1	1		2.099×10^{-1}	
		4	0.1	1		-2.074×10^{-1}	
		5	10.0	2		-7.751×10^{-4}	
		6	10.0	2		-6.283×10^{-5}	
		7	1.0	1		1.611×10^{-2}	
		8	1.0	1		-1.537×10^{-2}	

Note: [a]Multiple solutions of equal value are determined. See the text for these solutions

Table VI.
Values of parameters in the optimization algorithm

Total number of optimization runs	100
Genetic algorithm	
Population size	50
Mutation rate (%)	20
Elitism (%)	10
Parent percent used for offspring (%)	60
Number of iterations	70
Local search	
Maximum number of iterations	100

In Example 5, a number of different but equal mesh refinement combinations were determined 72 percent of the time using the hybrid algorithm. These combinations include: $\mathbf{m} = (1, 44, 1, 40)$; $\mathbf{m} = (1, 43, 1, 41)$; $\mathbf{m} = (1,42, 1, 42)$ determined in 20, 26 and 26 percent of the runs, respectively. All of these solutions result in a highly accurate



Notes: Initially $m_1 = 1$, $m_2 = 1$, $m_3 = 1$ and $m_4 = 1$. In the refined mesh $m_1 = 24$, $m_2 = 1$, $m_3 = 1$ and $m_4 = 1$

Figure 1.
Example 1

finite-element approximation to the convection-diffusion equation. The maximum errors associated with these discretizations are 2.153×10^{-8}, 9.996×10^{-9} and 1.300×10^{-9}, respectively. These results were reached in one to nine phase cycles of the hybrid search algorithm.

The hybrid algorithm results in a modest improvement over the direct search method in Example 4. One to two phase cycles of the hybrid search method were utilized to obtain these results. The direct search method determines an optimal solution of $\mathbf{m} = (2, 2, 2, 17)$ while the hybrid method determines the optimal solution to be $\mathbf{m} = (1, 1, 2, 17)$. The error associated with the improved hybrid solution is 1.669×10^{-8}.

Some of the optimal discretizations determined with the hybrid method for the example problems where $D = 5$ were obtained with the assistance of the adaptive abilities of the hybrid algorithm. To understand why the adaptive features of the hybrid algorithm were employed it is useful to examine the geometry of the feasible region for the optimization problem. For illustrative purposes the geometry of Example 4 is examined further.

Because the objective function is dependent upon m_1, m_2, m_3 and m_4, the relationship between the independent variables and the objective function cannot be fully viewed in one figure. By fixing $m_1 = 1$ and $m_2 = 1$ the feasible region of the objective function for Example 4 can be viewed as a function of m_3 and m_4 only (Figure 2). In Figure 2, the asterisks represent feasible solutions to the optimization problem. In this example problem the feasible region is separated into two regions that are not connected. The region where the optimal solution $\mathbf{m} = (1, 1, 2, 17)$ exists is very small compared to the region where suboptimal solutions exists. In some instances the hybrid algorithm fails to find the global optimal after one phase cycle because the feasible region is not connected and because the region where the global optimal exists is very small in the scope of the problem. By limiting the search space of the genetic algorithm in the second phase cycle of the hybrid algorithm, the likelihood of the random search method to determine a new feasible region is increased.

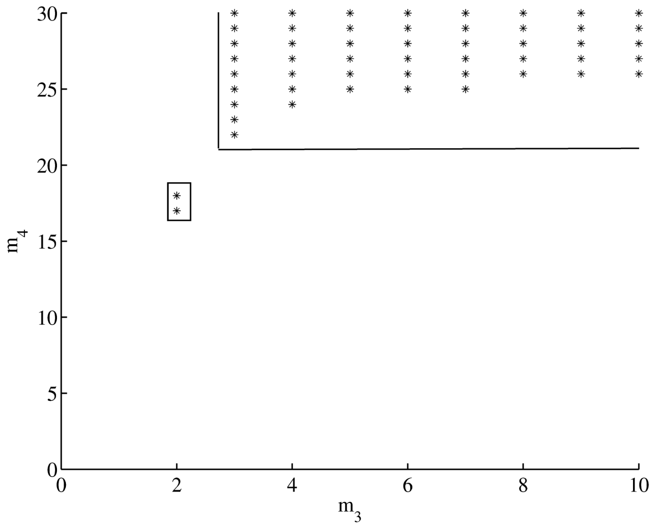


Figure 2.
Example 4

Notes: $m_1 = 1$, $m_2 = 1$. Asterisks represent feasible solutions and the boxes indicate connected feasible regions

The genetic algorithm employed in the hybrid method is a random start method and for this reason the likelihood of random combinations of m_i values falling within the region of the global optimal solution is quite small. The first phase cycle of the AGA successfully determines the large region where a feasible solution exists, and the local search successfully determines the local optimal solution within this region. The second phase cycle effectively locates the smaller feasible region where the global optimal solution exists by eliminating all but the boundary of the large feasible region from consideration in the genetic algorithm. Because of the random nature of the genetic algorithm and the potentially small sizes of the feasible regions that are not connected where globally optimal solutions may exist, it is possible that the AGA will not successfully locate truly optimal solutions. By limiting the search space of the AGA, the effectiveness of the algorithm is enhanced.

Example 4 clearly illustrates the benefits of using the multi-phase adaptive hybrid algorithm developed for this problem to determine a global optimal solution.

The results of the hybrid optimization algorithm for determining a minimal mesh refinement for Examples 7 through 12 are summarized in Table IV.

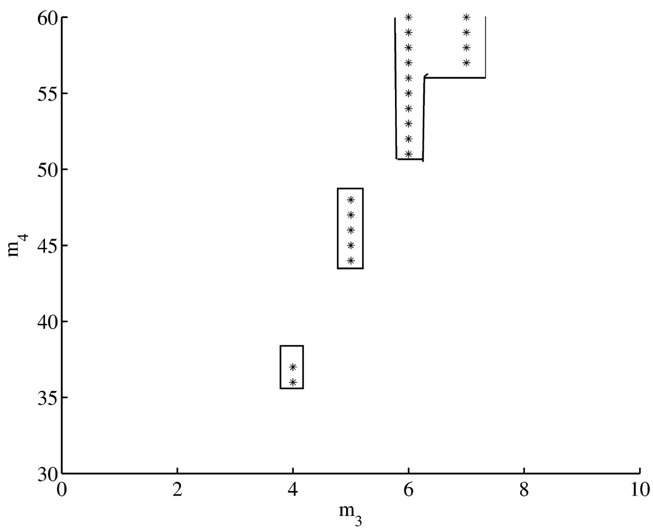
The results in Example 9 match the solution determined in the direct search method. In Example 9 the results were determined in one phase cycle of the hybrid algorithm. The solution for Example 9 is $\mathbf{m} = (1, 1, 54, 1)$ and was determined in 100 percent of the runs. The maximum error of the numerical solution given this discretizations is 1.776×10^{-15}.

The results from Examples 7, 8 and 12 are a great improvement over the direct search method. These results were determined after one phase cycle of the hybrid algorithm. The respective solutions for Example 7, 8 and 12 are $\mathbf{m} = (54, 1, 2, 1)$, $\mathbf{m} = (1, 54, 2, 1)$ and $\mathbf{m} = (1, 1, 54, 1)$, all obtained in 100 percent of the runs. The maximum errors of the numerical solutions to Examples 7 and 8 are 1.121×10^{-4} and 1.142×10^{-4}. The computer code that would generate the numerical solution given the discretization for Example 12 crashes due to unknown reasons.

In Example 11, a number of different but equal optimal mesh refinement combinations were determined 32% of the time using 1-11 phase cycles of the hybrid algorithm. These solutions are equal to the solution determined in the direct search method. The discretizations as well as the associated maximum errors in the numerical solutions include: $\mathbf{m} = (1, 145, 1, 139)$ with maximum error of 2.243×10^{-8}; $\mathbf{m} = (1, 144, 1, 140)$ with maximum error of 1.098×10^{-8}; $\mathbf{m} = (1, 143, 1, 141)$ with maximum error of 1.543×10^{-14}; $\mathbf{m} = (1, 142, 1, 142)$ with maximum error of 1.054×10^{-8}; $\mathbf{m} = (1, 141, 1, 143)$ with maximum error of 2.064×10^{-8}; $\mathbf{m} = (1, 140, 1, 144)$ with maximum error of 3.033×10^{-8}; and $\mathbf{m} = (1, 139, 1, 145)$ with maximum error of 3.962×10^{-8}. These refinements occur in 1, 7, 3, 4, 1, 6 and 10 percent of the runs so that the total number of equivalent solutions make up 32 percent of the runs.

Just as Example 4 was one such example for the $D = 5$ case where the hybrid algorithm required more than one phase cycle to determine a solution, so did the solution for Example 10 where $D = 1$. Between one and four phase cycles of the hybrid method were utilized to obtain the discretization of $\mathbf{m} = (1, 1, 4, 36)$ associated with a maximum error of 5.3291×10^{-15} in 91 percent of the runs. By fixing $m_1 = 1$ and $m_2 = 1$ the feasible region of the objective function is viewed as a function of m_3 and m_4 in Figure 3. Just as in Example 4, the feasible region for Example 10 is separated into regions that are not connected. In this example, there are three regions that are not connected, depicted in Figure 3. The adaptive hybrid method was able to locate the smallest of the three regions that are not connected where the global optimal feasible solution exists.

Examples 13 through 16 illustrate the ability of this hybrid algorithm to determine mesh refinements that result in accurate solutions to our convective-diffusion equation using the method of collocation with upstream or downstream weighting. These example problems contain elements of Examples 10 and 11. The characteristics of the objective functions for each of this problems is quite difficult to observe given that the dimensionality of the problems has risen from four to eight. The error analysis of



Notes: $m_1 = 1$, $m_2 = 1$. Asterisks represent feasible solutions and the boxes indicate connected feasible regions

Figure 3.
Example 10

the results, however, are perfectly reasonable to determine and are used as a measure of the effectiveness of the hybrid algorithm to determine reasonable results.

The results of the hybrid algorithm for Examples 13 through 16 are summarized in Table V. In Example 13 the hybrid method determines three equal solutions: $\mathbf{m} = (1, 1, 4, 59, 1, 2, 7, 63)$ with a maximum error of 5.854×10^{-12} in 4 percent of the runs; $\mathbf{m} = (1, 1, 4, 58, 1, 2, 7, 64)$ with a maximum error of 4.815×10^{-12} in 1 percent of the runs; $\mathbf{m} = (1, 1, 3, 53, 1, 2, 7, 55)$ with a maximum error of 1.815×10^{-11} in 1 percent of the runs. One to two phase cycles of the hybrid method were called to determine these solutions. While the equal discretizations determined above account for only 6 percent of the runs, it should be noted that the other 94 percent of the runs resulted in five different solutions that each contained just one more discretization refinement, for example $\mathbf{m} = (1, 1, 4, 62 ,1, 2, 7, 61)$.

In Example 14 the hybrid method determined the solution $\mathbf{m} = (1, 1, 1, 1, 4, 5, 44, 43)$ with a maximum error of 1.195×10^{-12} in 100 percent of the runs. One to four phase cycles were required in the optimization runs.

The hybrid method applied to Example 15 determined the equivalent solutions of $\mathbf{m} = (1, 1, 7, 1, 45, 1, 2, 1)$, $\mathbf{m} = (1, 1, 8, 1, 44, 1, 2, 1)$ and $\mathbf{m} = (1, 1, 9, 1, 43, 1, 2, 1)$ with maximum errors of 7.812×10^{-1}, 7.729×10^{-1} and 7.721×10^{-1}, respectively in 37, 20 and 13 percent of the runs for a total of 70 percent of the runs. One to eight phase cycles were employed in the hybrid method to obtain these solutions.

In Example 16 the hybrid method determined the solution $\mathbf{m} = (1, 38, 1, 1, 2, 2, 1, 1)$ with a maximum error of 9.436×10^{-1} in 100 percent of the runs. Only one phase cycle was required in all of the optimization runs.

7. Conclusions

To determine an optimal mesh refinement so that the method of collocation can determine highly accurate solutions to the steady-state one-dimensional convection-diffusion, one must solve a non-linear integer optimization problem. The results of this optimization problem provide both the mesh refinement as well as the upstream or downstream collocation locations for the convective term for each element of the finite-element mesh.

The constrained optimization problem was transformed into an unconstrained optimization problem. This was done by allowing violations of the constraints; however, when the violations occurred, the objective function was penalized. This transformation allowed for the application of a random search algorithm, namely a genetic algorithm. Refinement of the solution to the genetic algorithm was done through a newly developed local search technique designed to handle the variations in scale for this integer problem.

Due to possibility of feasible regions that are not connected in the presented optimization problem, an adaptive hybrid method was developed to solve this problem. The adaptive hybrid method utilizes both an AGA as well as a local GS technique developed specifically for this problem. This adaptive algorithm consisted of completing phase cycles of the AGA and the GS, with each cycle containing a search space that is limited by the results of the most recently completed phase cycle.

This adaptive hybrid method was successful at determining discretization solutions that were equal to or better than previous results determined through the direct search method. In cases where direct search methods have not been utilized to determine mesh refinements due to the high dimensionality of the problems, this method effectively determined mesh refinements that resulted in approximate solutions with reasonably small errors.

The geometry of the feasible regions of problems where multiple phase cycles were employed was examined. The results of this exploration indicate that in some instances this optimization problem is one with feasible regions that are not connected. In the two instances where the hybrid method utilized multiple phase cycles to determine a solution, the global optimal solution was found to be in a small region that is not connected. Because genetic algorithms are random search methods, the likelihood of finding the small regions that are not connected where the global optimal solution exists is dependent upon the size of the search space. The adaptive hybrid algorithm effectively determines feasible regions that are not connected because at each new phase cycle, the search space for the AGA is reduced, thereby increasing the likelihood of determining small feasible regions that are not connected where the optimal solution may exist.

There are two immediate extensions of this work that are possible. The first extension is that of determining accurate solutions to non-steady-state, one-dimensional advection-diffusion problems with time-dependent coefficients. Due to the variability of forms that these equations may take, it is difficult to generalize the solution determined through analytic methods to these equations. For these same reasons, it is not possible to determine a generalized form of solution determined through the method of collocation applied in this work. Without these two sets of solutions, it is not possible to determine an optimal discretization for all non-steady-state problems with time-dependent coefficients. For individual non-steady-state problems with time-dependent coefficients that are solvable using analytic methods, it is possible to extend this work directly as the solutions determined through the method of collocation can be derived for any problem. The first step to this extension, namely the non-steady-state problem with constant coefficients, is currently being developed for the non-steady-state problem.

The second immediate extension of this work is to examine how the method of collocation presented can be optimally accurate for a problem in a multi-dimensional velocity field. In general it is possible to solve the steady-state, advection-diffusion equation with constant coefficients using analytic methods. Determining the analytic solutions through the method of collocation, however, is a complicated problem and requires extensive work. Once these solutions have been derived, the optimization algorithm developed for this problem may be applied to determine minimal discretization for accurate solutions to the multi-dimensional problem.

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Appendix

To find ζ_k.

To determine a feasible ζ_k from m_k where k refers to the largest index of the largest v_i in the model, find the roots of the following polynomial, $G(\zeta_k)$:

$$G(\zeta_k) = [\beta_k - \beta_k \exp(\beta_k)]\zeta_k^2 + [4 + \beta_k - 4\exp(\beta_k) + \beta_k \exp(\beta_k)]\zeta_k + \frac{[\beta_k^2 + 6\beta_k + 12] - \exp(\beta_k)[\beta_k^2 - 6\beta_k + 12]}{6\beta_k}$$

In this equation β_i are the Peclet numbers for each element i and are functions of the mesh refinement of element i, m_i, the velocity prescribed to element i, v_i, the diffusion coefficient that is constant over the entire model, D and the maximum number on initial elements, p:

$$\beta_i = \frac{v_i}{Dpm_i}$$

To find ζ_i in terms of m_i, m_{i+1} and ζ_{i+1}.

To determine ζ_i in terms of m_i, m_{i+1} and ζ_{i+1}, find the roots of the following polynomial, $F(\zeta_i)$:

$$\begin{aligned} F(\zeta_i) = {} & B_{i+1}[(\beta_i^2 + 6\beta_i + 12 + 6\beta_i\zeta_i(4 + \beta_i + \beta_i\zeta_i))^{m_i}][\beta_i^2\zeta_i^2 + 4\beta_i\zeta_i + 2] \\ & - 2\beta_i p m_i][1 + \beta_i\zeta_i][(\beta_i^2 + 6\beta_i + 12 + 6\beta_i\zeta_i(4 + \beta_i + \beta_i\zeta_i))^{m_i}] \\ & - B_{i+1}[(\beta_i^2 - 6\beta_i + 12 + 6\beta_i\zeta_i(4 - \beta_i + \beta_i\zeta_i))^{m_i}][\beta_i^2\zeta_i^2 + 4\beta_i\zeta_i + 2] \end{aligned}$$

where

$$B_{i+1} = \frac{\left[\dfrac{\rho_{i+1}}{\lambda_{i+1}^{m_{i+1}} - 1}\right][\beta_i p m_i \exp(\beta_i m_i)]}{[\beta_{i+1} p m_{i+1} / \exp(\beta_{i+1} m_{i+1}) - 1][\exp(\beta_i m_i) - 1]}$$

and

$$\rho_{i+1} = \left[\frac{2\beta_{i+1}}{h_{i+1}}\right]\left[\frac{1+\beta_{i+1}\zeta_{i+1}}{\beta_{i+1}^2\zeta_{i+1}^2+4\beta_{i+1}\zeta_{i+1}+2}\right]$$

$$\lambda_{i+1} = \frac{\beta_{i+1}^2+6\beta_{i+1}+12+6\beta_{i+1}\zeta_{i+1}(4+\beta_{i+1}+\beta_{i+1}\zeta_{i+1})}{\beta_{i+1}^2-6\beta_{i+1}+12+6\beta_{i+1}\zeta_{i+1}(4-\beta_{i+1}+\beta_{i+1}\zeta_{i+1})}$$

To find ζ_{i+1} in terms of m_{i+1}, m_i and ζ_i.

To determine ζ_{i+1} in terms of m_{i+1}, m_i and ζ_i, find the roots of the following polynomial, $H(\zeta_{i+1})$:

$$\begin{aligned} H_i(\zeta_{i+1}) = {} & C_i[(\beta_{i+1}^2+6\beta_{i+1}+12+6\beta_{i+1}\zeta_{i+1} \\ & \times(4+\beta_{i+1}+\beta_{i+1}\zeta_{i+1}))^{m_{i+1}}][\beta_{i+1}^2\zeta_{i+1}^2+4\beta_{i+1}\zeta_{i+1}+2] \\ & -[\beta_{i+1}^2-6\beta_{i+1}+12+6\beta_{i+1}\zeta_{i+1} \\ & \times(4-\beta_{i+1}+\beta_{i+1}\zeta_{i+1})]^{m_{i+1}}\left[\frac{2\beta_{i+1}}{h_{i+1}}\right][1+\beta_{i+1}\zeta_{i+1}] \\ & -C_i[\beta_{i+1}^2-6\beta_{i+1}+12+6\beta_{i+1}\zeta_{i+1} \\ & \times(4-\beta_{i+1}+\beta_{i+1}\zeta_{i+1})]^{m_{i+1}}[\beta_{i+1}^2\zeta_{i+1}^2+4\beta_{i+1}\zeta_{i+1}+2] \end{aligned}$$

where

$$C_i = \frac{\left[\frac{\rho_i\lambda_i^{m_i}}{\lambda_i^{m_i}-1}\right][\beta_{i+1}pm_{i+1}]}{\left[\frac{\beta_i pm_i\exp(\beta_i m_i)}{\exp(\beta_i m_i)-1}\right][\exp(\beta_{i+1}m_{i+1})-1]}$$

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