



Recent Advancements to the Generalized High-Order Compact Scheme

ICIAM 2007 HOC Minisymposium

July 16-20, 2003

Bill Spatz

Sandia National Laboratories

with

Graham Carey

University of Texas at Austin

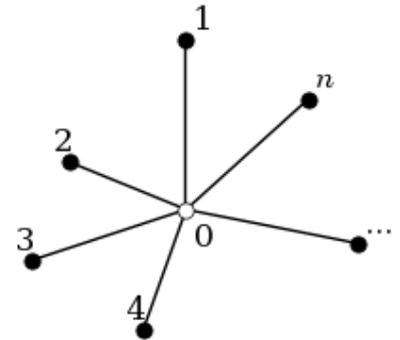


Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.



Background: GFDM

- Generalized Finite Difference Method (GFDM)
- Tworzydło, *IJNME*, 1988.
- Apply Taylor series approximations to unstructured grids
 - At each grid point, form a matrix system:



$$\begin{bmatrix} g_{10}^1 & g_{01}^1 & g_{20}^1 & g_{11}^1 & g_{02}^1 \\ g_{10}^2 & g_{01}^2 & g_{20}^2 & g_{11}^2 & g_{02}^2 \\ g_{10}^3 & g_{01}^3 & g_{20}^3 & g_{11}^3 & g_{02}^3 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ g_{10}^n & g_{01}^n & g_{20}^n & g_{11}^n & g_{02}^n \end{bmatrix} \begin{bmatrix} \phi_x \\ \phi_y \\ \phi_{xx} \\ \phi_{xy} \\ \phi_{yy} \end{bmatrix} \approx \begin{bmatrix} \phi_1 - \phi_0 \\ \phi_2 - \phi_0 \\ \phi_3 - \phi_0 \\ \vdots \\ \phi_n - \phi_0 \end{bmatrix}$$

$$g_{ij}^m = \frac{(x_m - x_0)^i (y_m - y_0)^j}{i! j!}$$

$$\mathbf{G}_0 \delta \phi_0 \approx \Delta \phi_0$$



Background: GFDM

- If this G_0 is invertible ($n=5$, restricted colinearity of grid points), then we can obtain stencil matrix $S_0=G_0^{-1}$:

$$\begin{bmatrix} \phi_x \\ \phi_y \\ \phi_{xx} \\ \phi_{xy} \\ \phi_{yy} \end{bmatrix}_0 \approx \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} \\ S_{21} & S_{22} & S_{23} & S_{24} & S_{25} \\ S_{31} & S_{32} & S_{33} & S_{34} & S_{35} \\ S_{41} & S_{42} & S_{43} & S_{44} & S_{45} \\ S_{51} & S_{52} & S_{53} & S_{54} & S_{55} \end{bmatrix}_0 \begin{bmatrix} \phi_1 - \phi_0 \\ \phi_2 - \phi_0 \\ \phi_3 - \phi_0 \\ \phi_4 - \phi_0 \\ \phi_5 - \phi_0 \end{bmatrix}$$

- If $n < 5$, then system is under-specified \rightarrow invalid grid

Background: GFDM

- If $n > 5$, system is over-specified \rightarrow one option is to use linear least-squares: $S_0 = (G_0^T G_0)^{-1} G_0$
- *Special case*: structured grid aligned with coordinate system $\rightarrow n=4$, but G_0 is given by

$$G_0 = \begin{bmatrix} (x_1 - x_0) & 0 & (x_1 - x_0)^2 / 2 & 0 & 0 \\ 0 & (y_2 - y_0) & 0 & 0 & (y_2 - y_0)^2 / 2 \\ (x_3 - x_0) & 0 & (x_3 - x_0)^2 / 2 & 0 & 0 \\ 0 & (y_4 - y_0) & 0 & 0 & (y_4 - y_0)^2 / 2 \end{bmatrix}$$

- We can eliminate column 4 and ϕ_{xy} from $\delta\phi_0$ to obtain an invertible 4×4 system.



Recap of GFDM

- For every grid point, we build a Taylor series matrix G_0 .
- For every G_0 , we obtain a stencil matrix S_0 (either G_0^{-1} or $(G_0^T G_0)^{-1} G_0$), which gives us a way to compute or express the derivatives of variables at each grid point.
- These expressions for derivatives can be used to build a global system to solve the governing PDE(s).



Generalized High-Order Compact Scheme

- **Question:** can we combine the ideas of high-order compact schemes and the GFDM?
- **Proposed approach:**
 - Extend $\delta\phi_0$ to include additional derivatives (typically through order 4).
 - Additional columns of G_0 can be obtained from Taylor series coefficients.
 - This forces the need for additional rows to obtain an invertible system.
 - Improve compactness by filling new rows of G_0 with derivatives of governing or auxiliary equations.
 - **Aside:** nonlinear problems would require solution of the G_0 operators at every iterate/time-step.

Simple 1D GHOC Example

- **1D convection-diffusion**

$$-\phi_{xx} + c\phi_x = f(x) \text{ on } x \in [0..1],$$

$$\text{with } \phi(0) = 0, \phi(1) = 1.$$

- **1D, nonuniform grid $\{x_i\}$, GHOC system:**

$$\begin{bmatrix} (x_{i-1} - x_i) & (x_{i-1} - x_i)^2 / 2 & (x_{i-1} - x_i)^3 / 6 & (x_{i-1} - x_i)^4 / 24 \\ (x_{i+1} - x_i) & (x_{i+1} - x_i)^2 / 2 & (x_{i+1} - x_i)^3 / 6 & (x_{i+1} - x_i)^4 / 24 \\ 0 & c & -1 & 0 \\ 0 & 0 & c & -1 \end{bmatrix} \begin{bmatrix} \phi_x \\ \phi_{xx} \\ \phi_{xxx} \\ \phi_{xxxx} \end{bmatrix}_i \approx \begin{bmatrix} \phi_{i-1} - \phi_i \\ \phi_{i+1} - \phi_i \\ f_x \\ f_{xx} \end{bmatrix}_i$$

- **Derivatives of $f(x)$ can be obtained with GFDM.**

1D GHOC for General Linear Equation

- The simplicity of the last two rows inspires more generalization:

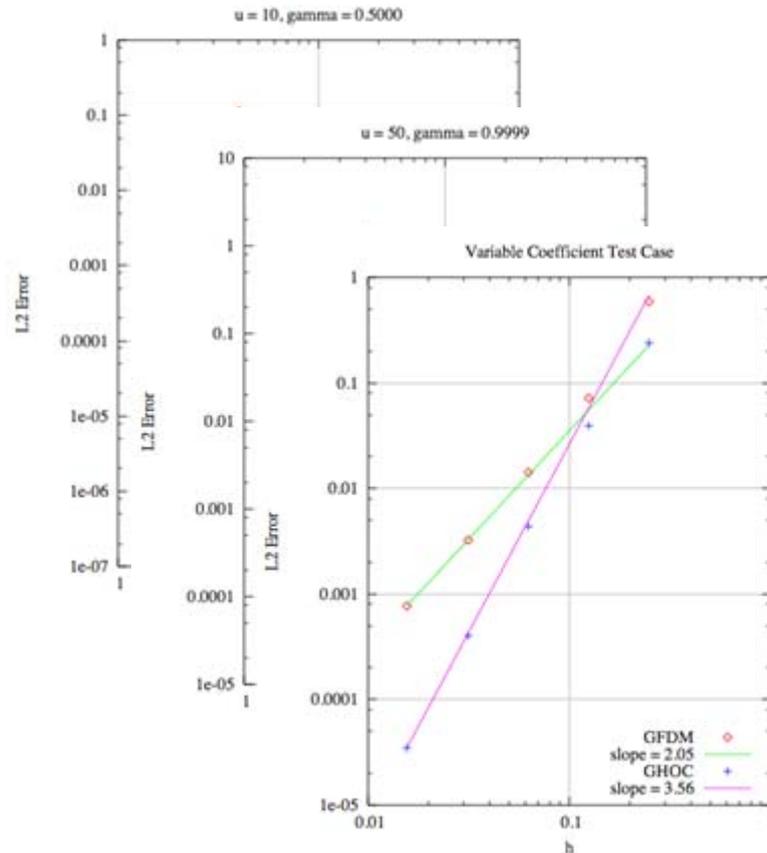
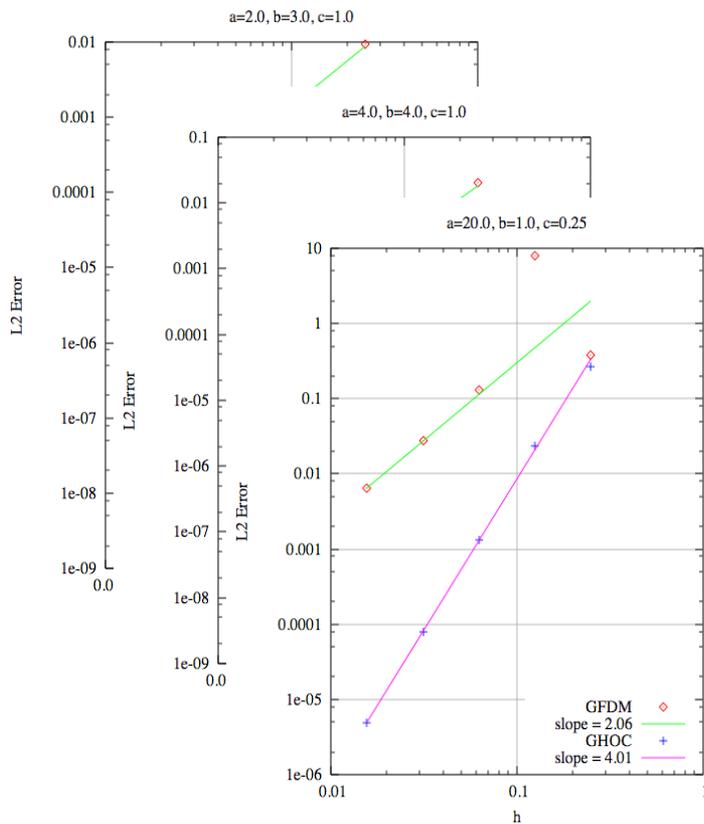
$$a(x)\phi + b(x)\phi_x + c(x)\phi_{xx} = f(x)$$

- Yields GHOC system:

$$\begin{bmatrix} (x_{i-1} - x_i) & (x_{i-1} - x_i)^2 / 2 & (x_{i-1} - x_i)^3 / 6 & (x_{i-1} - x_i)^4 / 24 \\ (x_{i+1} - x_i) & (x_{i+1} - x_i)^2 / 2 & (x_{i+1} - x_i)^3 / 6 & (x_{i+1} - x_i)^4 / 24 \\ a + b_x & b + c_x & c & 0 \\ 2a_x + b_{xx} & a + 2b_x + c_{xx} & b + 2c_x & c \end{bmatrix} \begin{bmatrix} \phi_x \\ \phi_{xx} \\ \phi_{xxx} \\ \phi_{xxxx} \end{bmatrix}_i = \begin{bmatrix} \phi_{i-1} - \phi_i \\ \phi_{i+1} - \phi_i \\ f_x - a_x \phi_i \\ f_{xx} - a_{xx} \phi_i \end{bmatrix}_i$$

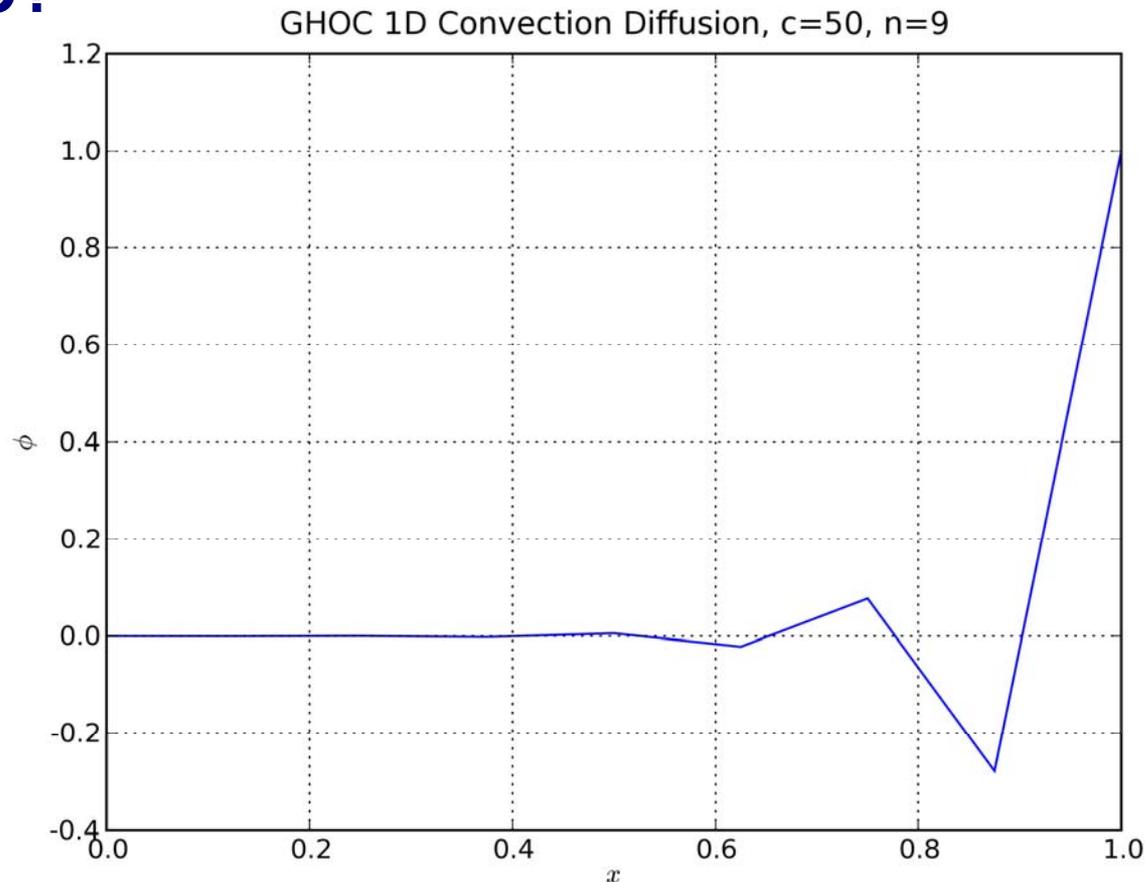
1D GHOC Convergence Results

- Previous results verify 4th-order accuracy:



1D GHOC vs Classic HOC

- Is GHOC on a uniform grid the same as classic HOC?



Analysis of Simple 1D GHOC

- If GHOC is not classic HOC, what is it?
- We can study GHOC system, restricted to simple convection-diffusion (constant $c, f=0$) on a uniform grid, to obtain the answer.
- Apply Gaussian elimination to obtain

$$\begin{bmatrix} h & h^2/2 & h^3/6 & h^4/24 \\ 0 & h^2 & 0 & h^4/12 \\ 0 & 0 & h^2 & ch^4/12 \\ 0 & 0 & 0 & h^2(1+c^2h^2/12) \end{bmatrix} \begin{bmatrix} \phi_x \\ \phi_{xx} \\ \phi_{xxx} \\ \phi_{xxxx} \end{bmatrix}_i \approx \begin{bmatrix} \phi_{i-1} - \phi_i \\ \phi_{i+1} - 2\phi_i + \phi_{i-1} \\ c(\phi_{i+1} - 2\phi_i + \phi_{i-1}) \\ c^2(\phi_{i+1} - 2\phi_i + \phi_{i-1}) \end{bmatrix}$$

- Solve for derivatives:

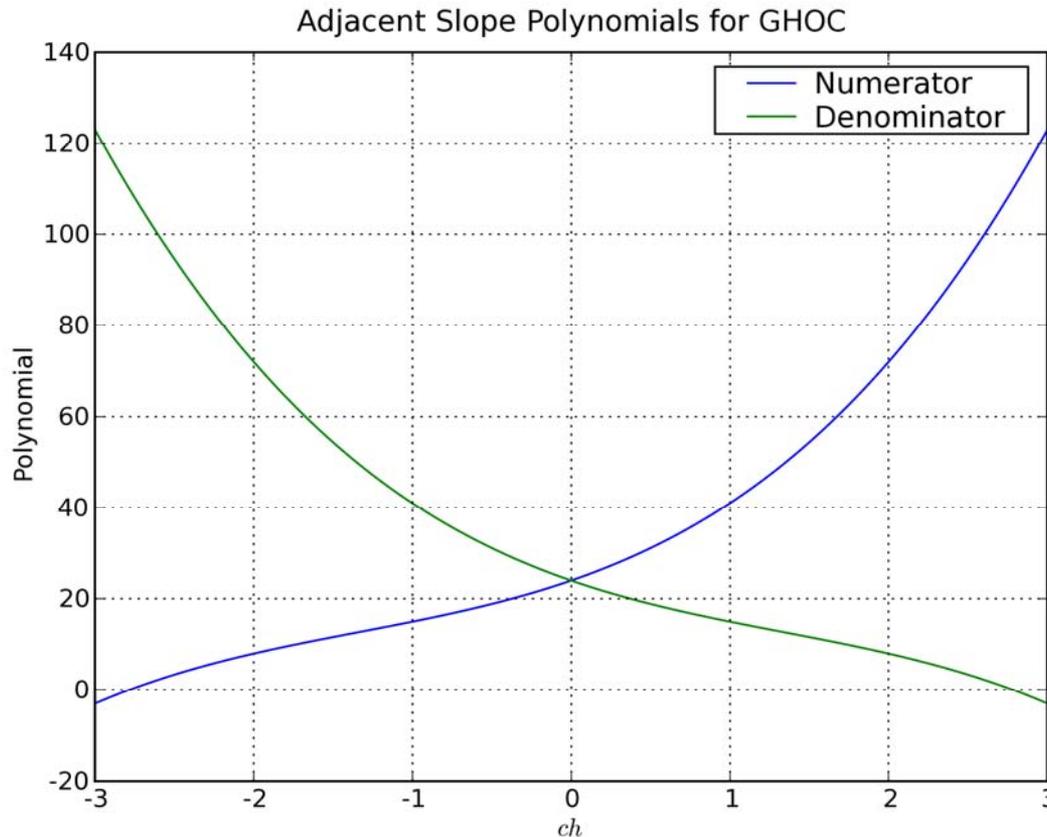
$$(\phi_x)_i \approx \delta_x \phi_i - \frac{2ch^2}{12+c^2h^2} \delta_x^2 \phi_i,$$

$$(\phi_{xx})_i \approx \frac{12}{12+c^2h^2} \delta_x^2 \phi_i.$$

Cell-Peclet Condition for 1D GHOC

- Plug these into governing equation and solve for ratio of adjoining slopes:

$$\frac{(\phi_{i+1} - \phi_i)/h}{(\phi_i - \phi_{i-1})/h} = \frac{c^3 h^3 + 4c^2 h^2 + 12ch + 24}{-c^3 h^3 + 4c^2 h^2 - 12ch + 24}$$



- Roots (Cardano's method):

$$ch = \pm 2.9132412572848\dots$$

2D GHOC: Poisson's Equation

$$\nabla^2 \phi = f(x, y)$$

- Extend $\delta\phi_0$: (2 first derivatives + 3 second derivatives + 4 third derivatives + 5 fourth derivatives) = **14** elements in vector.
- Take derivatives of governing equation: (x, y, xx, xy, yy) = **5** rows.
- For an invertible system, we need $(14-5)$ = **9** grid points in our stencil.
- Applying to a structured grid, we only have **8** neighboring grid points \rightarrow have to play some kind of game to get a well-defined stencil.

ϕ_x
 ϕ_y
 ϕ_{xx}
 ϕ_{xy}
 ϕ_{yy}
 ϕ_{xxx}
 ϕ_{xxy}
 ϕ_{xyy}
 ϕ_{yyy}
 ϕ_{xxxx}
 ϕ_{xxxy}
 ϕ_{xxyy}
 ϕ_{xyyy}
 ϕ_{yyyy}



Conclusions

- Have extended **GFDM** to include **HOC** ideas
 - Transferred tedious part of derivation to the computer
- **One dimension**
 - Applied to completely general linear BVP
 - Nonuniform grids handled automatically
 - Fourth order convergence (demonstrated)
 - GHOC is *different* than classic HOC
- **Two dimensions**
 - Better understanding of matrix rank for standard, 9-point, orthogonal stencil
- **Other extensions:**
 - Time dependent: $f = S(x) - \partial\phi/\partial t$
 - Three dimensions
 - Nonlinear