

Nonlinear Computational Methods for Simulating Interactions of Radiation with Matter in Physical Systems

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Introduction

- The simulation of interaction of particles with matter is a challenging problem.
- The transport equation is a basis for mathematical models of this physical phenomenon.
- Transport problems are difficult to solve
 - high dimensionality,
 - an integro-differential equation,
 - coefficients depend on the state of matter \iff the state of matter is affected by fluxes of particles.
- Applications:
 - reactor physics,
 - astrophysics (stars),
 - plasma physics (laser fusion),
 - atmospheric sciences.

Introduction

- There exists a family of efficient nonlinear methods for solving the transport equation:
Quasidiffusion method (V. Gol'din, 1964),
Nonlinear Diffusion Acceleration (K. Smith, 2002),
Flux methods (T. Germogenova, V. Gol'din, 1969).
- These methods are defined by a system of nonlinearly coupled high-order and low-order problems that is equivalent to the original linear transport problem.
- The Nonlinear Projective Iteration (NPI) methods possess certain advantages for their use in multiphysics applications.
- The low-order equations of NPI methods can be used to formulate approximate particle transport models.
- These low-order equations can also be utilized as a basis for development of hybrid Monte Carlo computational methods.
- The NPI methods are distinct from each other by the definition of the low-order equations which gives rise to differences in features of these methods.

Introduction

- Outline
 - A Tutorial on nonlinear methods for solving the transport equation
 - The Quasidiffusion (QD) method for transport problems in 2D Cartesian geometry on grids composed of arbitrary quadrilaterals
 - Nonlinear Weighted Flux (NWF) methods for particle transport problems in 2D Cartesian geometry on orthogonal grid
- This work was performed in collaboration with my Ph.D. students at NCSU
 - William A. Wieselquist (to graduate in 2008 → Paul Scherrer Institute, Switzerland)
 - Loren Roberts (graduated in 2008 → Baker Hughes Inc.)

Transport Problem

- Let us consider the following single-group slab geometry transport problem with isotropic scattering and source:

$$\mu \frac{\partial}{\partial x} \psi(x, \mu) + \Sigma_t(x) \psi(x, \mu) = \frac{1}{2} \left(\Sigma_s(x) \int_{-1}^1 \psi(x, \mu') d\mu' + Q(x) \right) ,$$

$$-1 \leq \mu \leq 1 , \quad 0 \leq x \leq L ,$$

$$\phi(x) = \int_{-1}^1 \psi(x, \mu) d\mu , \quad J(x) = \int_{-1}^1 \mu \psi(x, \mu) d\mu ,$$

with reflective left boundary

$$\psi(0, \mu) = \psi(0, -\mu) , \quad 0 < \mu \leq 1 ,$$

and vacuum boundary condition on the right

$$\psi(L, \mu) = 0 , \quad -1 \leq \mu < 0 .$$

Low-Order Equations

- The transport equation is integrated over $-1 \leq \mu \leq 1$ with weights 1 and μ

$$\frac{dJ}{dx} + (\Sigma_t - \Sigma_s)\phi = Q,$$

$$\frac{d}{dx} \left(\int_{-1}^1 \mu^2 \psi d\mu \right) + \Sigma_t J = 0,$$

where

$$\phi(x) = \int_{-1}^1 \psi(x, \mu) d\mu, \quad J(x) = \int_{-1}^1 \mu \psi(x, \mu) d\mu.$$

- What should we do with the extra moment?

$$\int_{-1}^1 \mu^2 \psi d\mu = ?$$

Approximate Closure: Diffusion Theory

- Diffusion theory (approximation)

$$\psi(x, \mu) = \frac{1}{2}(\phi(x) + 3\mu J(x)) ,$$

$$\int_{-1}^1 \mu^2 \psi d\mu = \frac{1}{3} \phi(x) .$$

- P₁ equations

$$\frac{dJ}{dx} + (\Sigma_t - \Sigma_s)\phi = Q ,$$

$$\frac{1}{3} \frac{d\phi}{dx} + \Sigma_t J = 0 ,$$

- Diffusion equation

$$-\frac{d}{dx} \frac{1}{3\Sigma_t} \frac{d\phi}{dx} + (\Sigma_t - \Sigma_s)\phi = Q ,$$

Approximate Closure: Variable Eddington Factor Method

$$\int_{-1}^1 \mu^2 \psi d\mu \approx \mathcal{F}(x) \phi(x)$$

- Minerbo closure (approximation)

$$\psi(x, \mu) = \alpha(x) e^{\mu\beta(x)} \quad \mathcal{F}(x) = 1 - \frac{2}{Z(x)} \frac{|J(x)|}{\phi(x)},$$

- Kershaw closure (approximation)

$$\mathcal{F}(x) = \frac{1}{3} \left(1 + 2 \left(\frac{|J(x)|}{\phi(x)} \right)^2 \right)$$

- Levermore-Pomraning closure (approximation)

$$\mathcal{F}(x) = \frac{|J(x)|}{\phi(x)} \coth(Z(x)), \quad \coth(Z) - \frac{1}{Z} = \frac{|J|}{\phi}$$

- P₁-like nonlinear low-order equations

$$\frac{dJ}{dx} + (\Sigma_t - \Sigma_s) \phi = Q,$$

$$\frac{d}{dx}(\mathcal{F}\phi) + \Sigma_t J = 0, \quad \mathcal{F} = \mathcal{F}(\phi, J)$$

Quasidiffusion (QD) Method: Exact Closure

- The Quasidiffusion method (exact)

$$\int_{-1}^1 \mu^2 \psi d\mu = \left[\frac{\int_{-1}^1 \mu^2 \psi d\mu}{\int_{-1}^1 \psi d\mu} \right] \int_{-1}^1 \psi d\mu = E(x) \phi(x),$$

- The quasidiffusion factor.

$$E(x) = \frac{\int_{-1}^1 \mu^2 \psi d\mu}{\int_{-1}^1 \psi d\mu} = \langle \mu^2 \rangle$$

- Quasidiffusion low-order equations

$$\frac{dJ}{dx} + (\Sigma_t - \Sigma_s) \phi = Q,$$

$$\frac{dE\phi}{dx} + \Sigma_t J = 0, \quad E = E[\psi].$$

System of Equations of the Quasidiffusion (QD) Method

- The transport (high-order) equation

$$\mu \frac{\partial}{\partial x} \psi(x, \mu) + \Sigma_t \psi(x, \mu) = \frac{1}{2} (\Sigma_s \phi(x) + Q).$$

- QD (variable Eddington) factors

$$E(x) = \frac{\int_{-1}^1 \mu^2 \psi(x, \mu) d\mu}{\int_{-1}^1 \psi(x, \mu) d\mu}, \quad C_L = \frac{\int_{-1}^0 \mu \psi(L, \mu) d\mu}{\int_{-1}^0 \psi(L, \mu) d\mu}.$$

- the low-order QD equations

$$\frac{d}{dx} J(x) + (\Sigma_t - \Sigma_s) \phi(x) = Q,$$

$$\frac{d}{dx} \left(E(x) \phi(x) \right) + \Sigma_t J(x) = 0.$$

$$J(0) = 0,$$

$$J(L) = C_L \phi(L).$$

QD Method: Iteration Process

- High-order problem (transport sweep)

$$\mu \frac{\partial}{\partial x} \psi^{(s+1/2)} + \Sigma_t \psi^{(s+1/2)} = \frac{1}{2} (\Sigma_s \phi^{(s)} + Q),$$

- Calculation of QD factors

$$E^{(s+1/2)}(x) = \frac{\int_{-1}^1 \mu^2 \psi^{(s+1/2)}(x, \mu) d\mu}{\int_{-1}^1 \psi^{(s+1/2)}(x, \mu) d\mu}, \quad C_L = \frac{\int_{-1}^0 \mu \psi^{(s+1/2)}(L, \mu) d\mu}{\int_{-1}^0 \psi^{(s+1/2)}(L, \mu) d\mu}.$$

- Low-order QD problem

$$\frac{d}{dx} J^{(s+1)} + (\Sigma_t - \Sigma_s) \phi^{(s+1)} = Q,$$

$$\frac{d}{dx} \left(E^{(s+1/2)} \phi^{(s+1)} \right) + \Sigma_t J^{(s+1)} = 0,$$

$$J^{(s+1)}(0) = 0,$$

$$J^{(s+1)}(L) = C_L^{(s+1/2)} \phi^{(s+1)}(L).$$

Nonlinear Diffusion Acceleration (NDA)

(Kord Smith)

- High-order problem (transport sweep)

$$\mu \frac{\partial}{\partial x} \psi^{(s+1/2)} + \Sigma_t \psi^{(s+1/2)} = \frac{1}{2} (\Sigma_s \phi^{(s)} + Q) ,$$

- Calculation of $\tilde{\mathcal{D}}^{(s+1/2)}$

$$J^{(s+1/2)}(x) = \int_{-1}^1 \mu \psi^{(s+1/2)}(x, \mu) d\mu , \quad \phi^{(s+1/2)}(x) = \int_{-1}^1 \psi^{(s+1/2)}(x, \mu) d\mu ,$$

$$\tilde{\mathcal{D}}^{(s+1/2)} = -\frac{1}{\phi^{(s+1/2)}} \left(J^{(s+1/2)} + \frac{1}{3\Sigma_t} \frac{d\phi^{(s+1/2)}}{dx} \right) .$$

- Low-order NDA problem

$$\frac{d}{dx} J^{(s+1)} + (\Sigma_t - \Sigma_s) \phi^{(s+1)} = Q ,$$

$$\frac{1}{3\Sigma_t} \frac{d\phi^{(s+1)}}{dx} + \tilde{\mathcal{D}}^{(s+1/2)} \phi^{(s+1)} + J^{(s+1)} = 0 ,$$

QD Method for the Multidimensional Transport Equation

- The transport (high-order) equation

$$\vec{\Omega} \cdot \vec{\nabla} \psi^{(k+1/2)}(\vec{r}, \vec{\Omega}) + \sigma_t(\vec{r}) \psi^{(k+1/2)}(\vec{r}, \vec{\Omega}) = \frac{1}{4\pi} \sigma_s(\vec{r}) \phi^{(k)}(\vec{r}) + \frac{1}{4\pi} q(\vec{r}).$$

- The QD (Eddington) tensor

$$\bar{\bar{E}} = \begin{pmatrix} E_{xx} & E_{xy} \\ E_{xy} & E_{yy} \end{pmatrix},$$

$$E_{\alpha\beta}^{(k+1/2)}(\vec{r}) = \int_{4\pi} \Omega_\alpha \Omega_\beta \psi^{(k+1/2)}(\vec{r}, \vec{\Omega}) d\vec{\Omega} \Big/ \int_{4\pi} \psi^{(k+1/2)}(\vec{r}, \vec{\Omega}) d\vec{\Omega}, \quad \alpha, \beta = x, y,$$

$$E_{\alpha\beta}(\vec{r}) = \text{average value of } \Omega_\alpha \Omega_\beta.$$

- The low-order QD (LOQD) equations

$$\vec{\nabla} \cdot \vec{J}^{(k+1)}(\vec{r}) + \sigma_a(\vec{r}) \phi^{(k+1)}(\vec{r}) = q(\vec{r}),$$

$$\vec{J}^{(k+1)}(\vec{r}) = -\frac{1}{\sigma_t(\vec{r})} \vec{\nabla} \cdot \left(\bar{\bar{E}}^{(k+1/2)}(\vec{r}) \phi^{(k+1)}(\vec{r}) \right).$$

Discretization of the LOQD Equations

- The unknowns: ϕ_i , $\phi_{i\omega}$, and $J_{i\omega} = \vec{J}_{i\omega} \cdot \vec{n}_{i\omega}$,
- The balance equation in i th cell

$$\sum_{\omega} \vec{J}_{i\omega} \cdot \vec{A}_{i\omega} + \sigma_{a,i} \phi_i V_i = q_i V_i, \quad \text{where } \omega - \text{cell face.}$$

- Jim Morel (2002) proposed a cell-centered discretization for the diffusion equation on meshes of arbitrary polyhedrons.

$$\{\vec{\nabla} \phi\}_{i\omega} = (\phi_{i\omega} - \phi_i) \vec{\alpha}_{i\omega} + \frac{1}{V_i} \sum_{\omega'} (\phi_{i\omega'}) \vec{\beta}_{i\omega\omega'},$$

where $\vec{\alpha}_{i\omega}$ and $\vec{\beta}_{i\omega\omega'}$ are based on geometry.

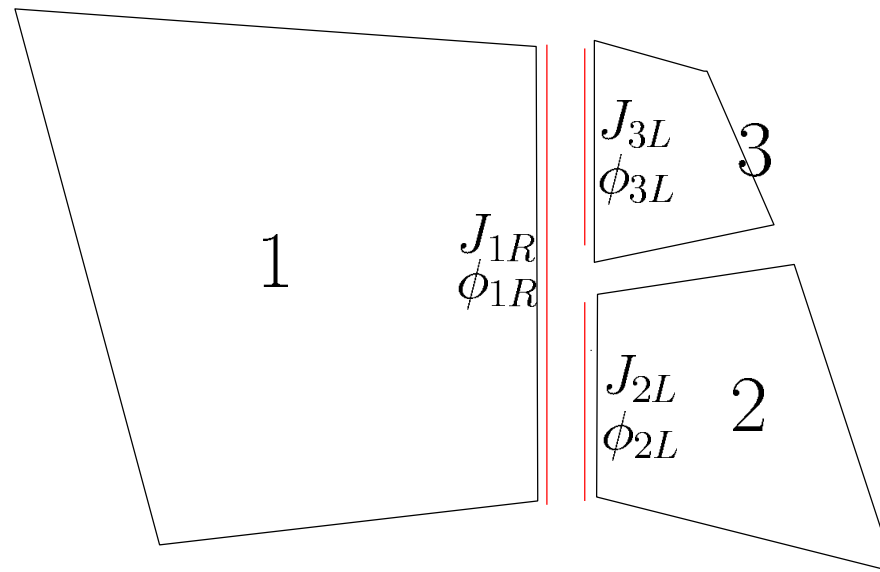
- We apply Morel's method

$$\vec{J}_{i\omega} = -\frac{1}{\sigma_{t,i}} \left\{ \vec{\nabla} \cdot (\vec{E} \phi) \right\}_{i\omega}.$$

$$\left\{ \vec{\nabla} \cdot (\vec{E} \phi) \right\}_{i\omega} = \vec{e}_x \left(\left\{ \frac{\partial E_{xx} \phi}{\partial x} \right\}_{i\omega} + \left\{ \frac{\partial E_{xy} \phi}{\partial y} \right\}_{i\omega} \right) + \vec{e}_y \left(\left\{ \frac{\partial E_{xy} \phi}{\partial x} \right\}_{i\omega} + \left\{ \frac{\partial E_{yy} \phi}{\partial y} \right\}_{i\omega} \right).$$

Discretization of the LOQD Equations

- Conditions at interfaces between cells



- Strong current and weak scalar flux continuity conditions

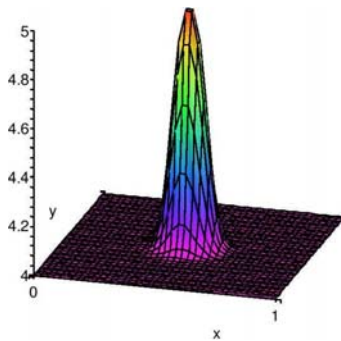
$$\begin{aligned}J_R &= -J_{2L} \\J_R &= -J_{3L} \\ \phi_R A_R &= \phi_{2L} A_{2L} + \phi_{3L} A_{3L}\end{aligned}$$

Analytic Test Problem for the LOQD Equations

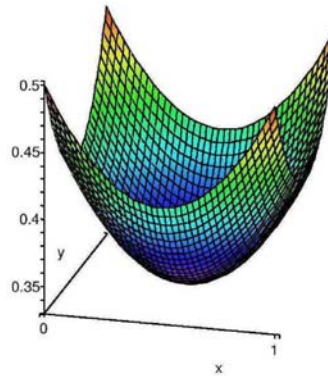
- $0 \leq x \leq 1$, $0 \leq y \leq 1$. $\sigma_t = 1$, $\sigma_a = 0.5$.
- Analytic solution

$$\phi(x, y) = 5 - \tanh \left[100 \left(x - \frac{1}{2} \right)^2 + 100 \left(y - \frac{1}{2} \right)^2 \right]$$

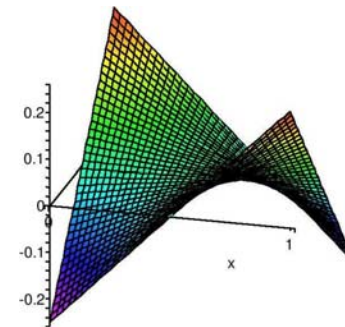
- The QD tensor ($E_{\alpha\beta}(x, y)$) is given in analytic form



$\phi(x, y)$



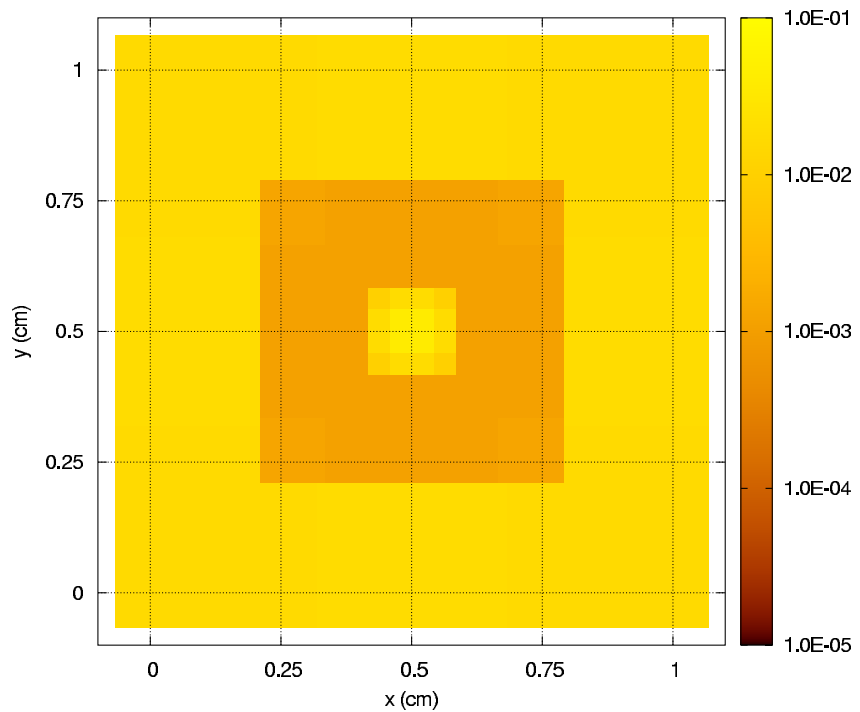
$E_{xx}(x, y)$



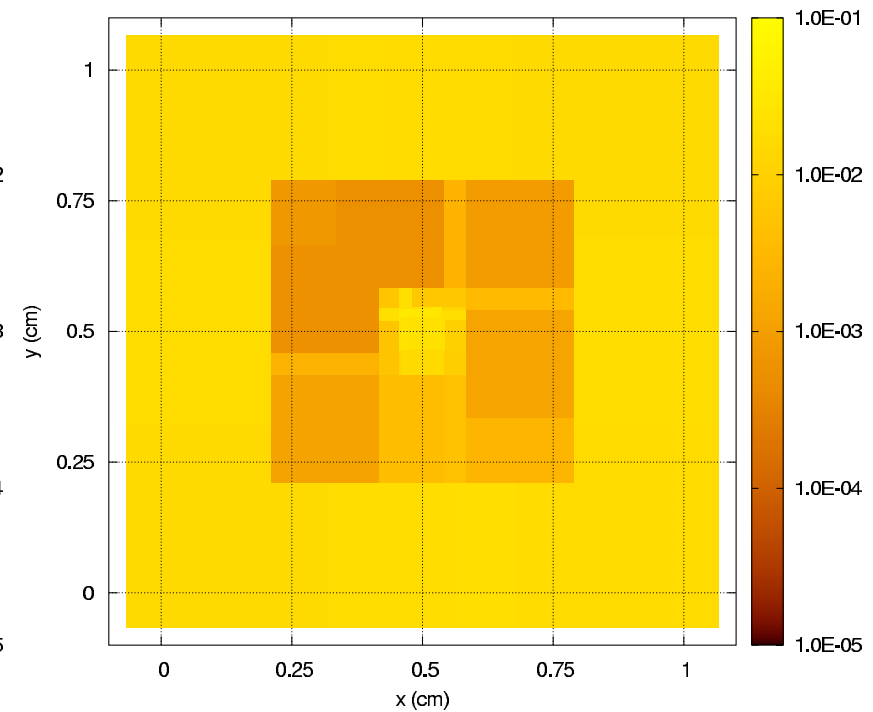
$E_{xy}(x, y)$

Results on 3-Level Grids

- Relative error in the cell-average scalar flux
- Grid 1: 40 cells



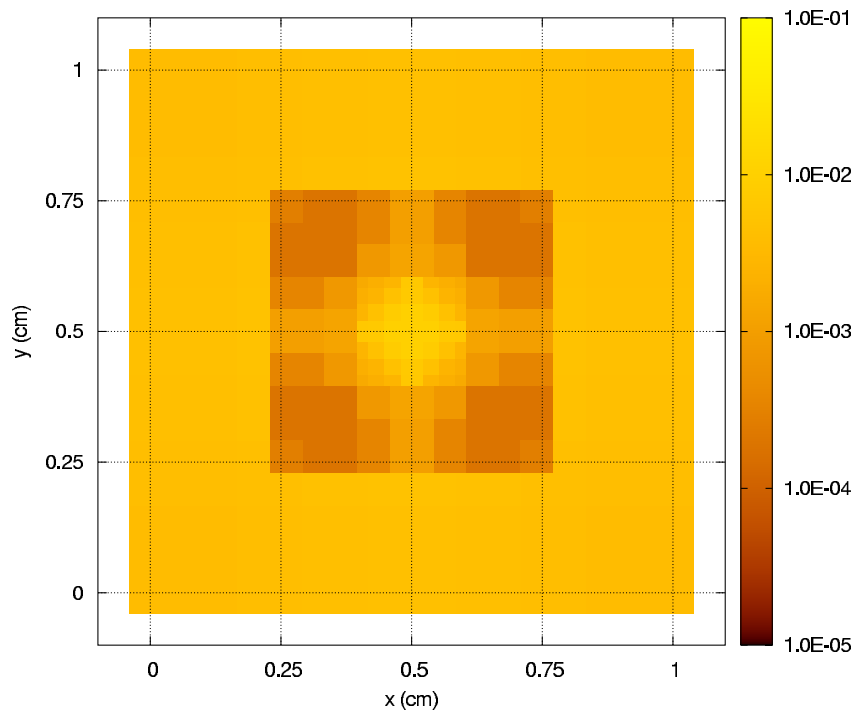
orthogonal grid



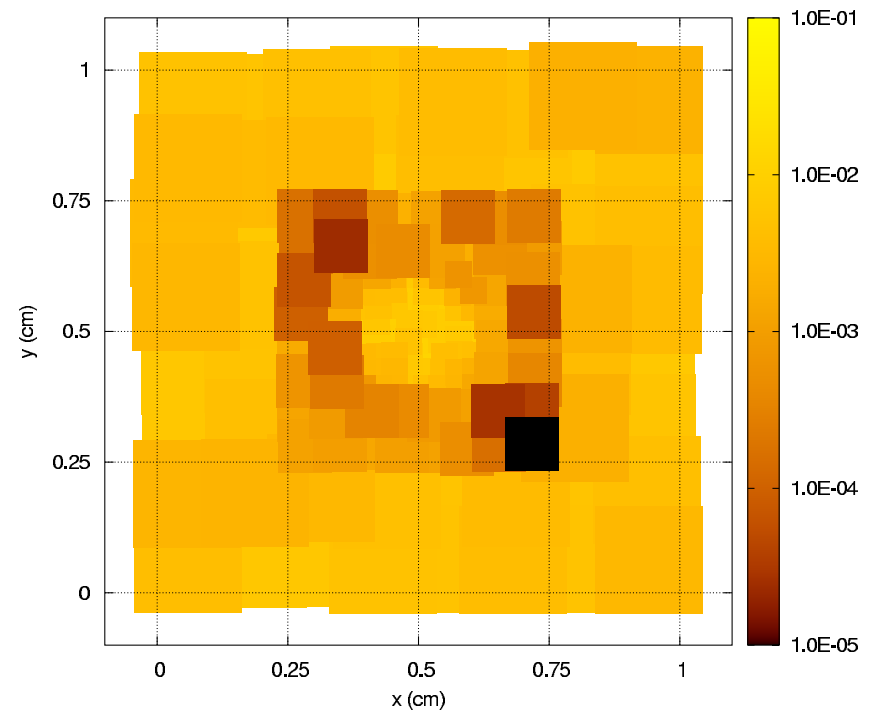
randomized (20%) grid

Results on 3-Level Grids

- Relative error in the cell-average scalar flux
- Grid 2: 160 cells



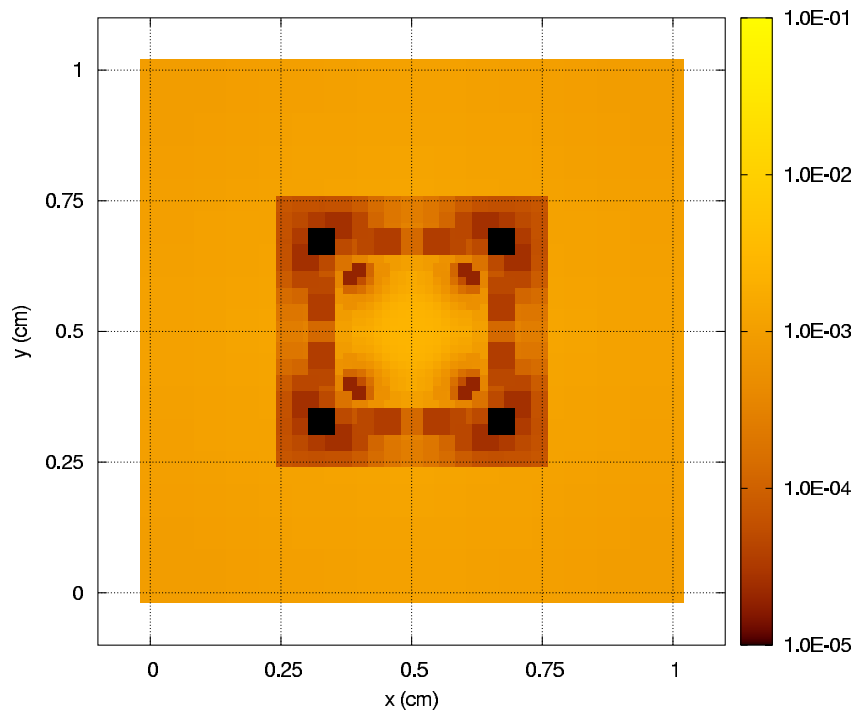
orthogonal grid



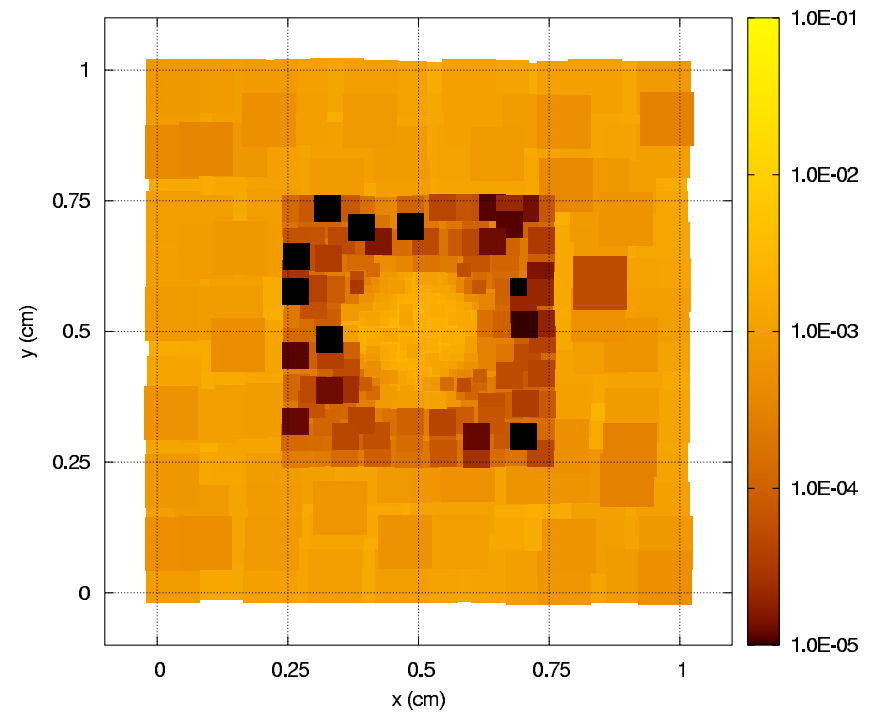
randomized (20%) grid

Results on 3-Level Grids

- Relative error in the cell-average scalar flux
- Grid 3: 640 cells



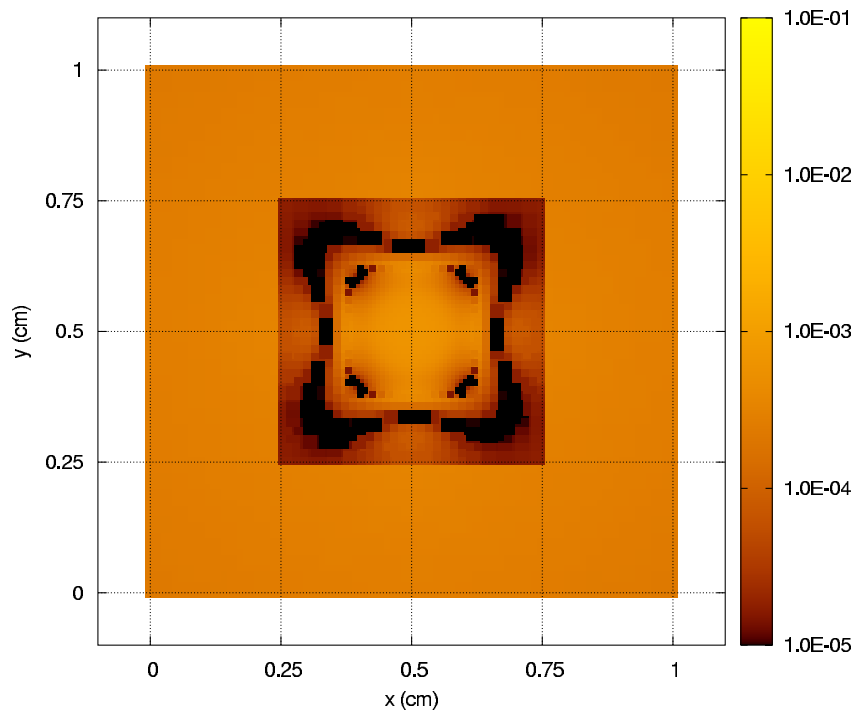
orthogonal grid



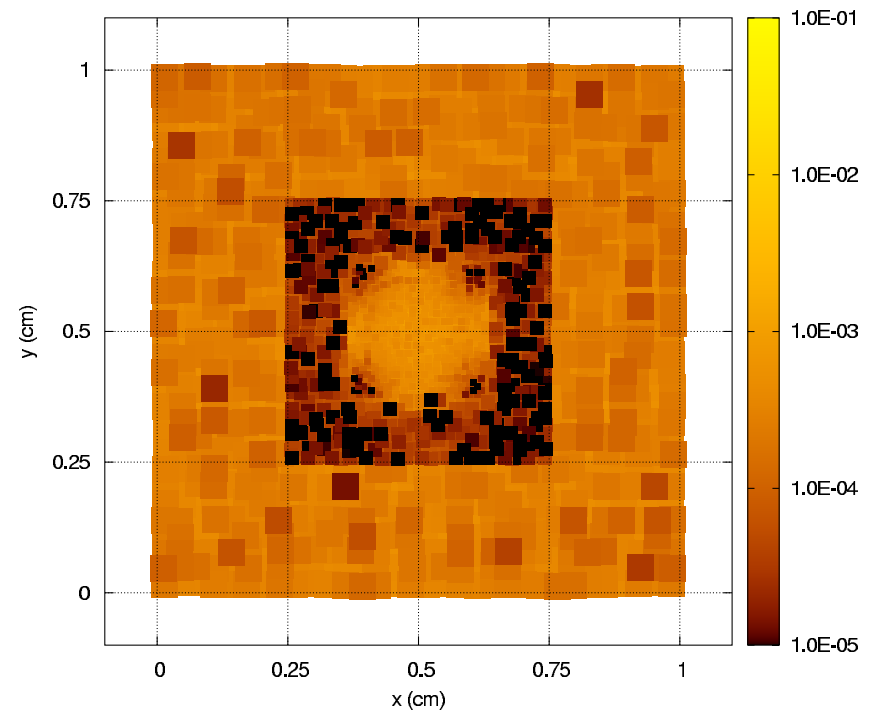
randomized (20%) grid

Results on 3-Level Grids

- Relative error in the cell-average scalar flux
- Grid 4: 2560 cells

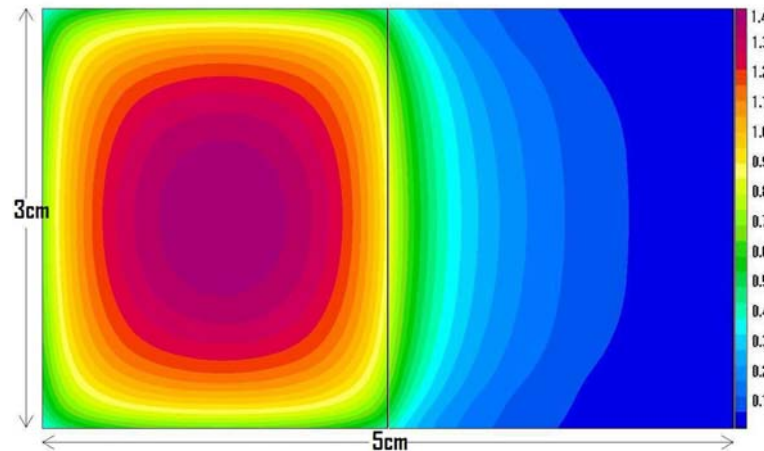
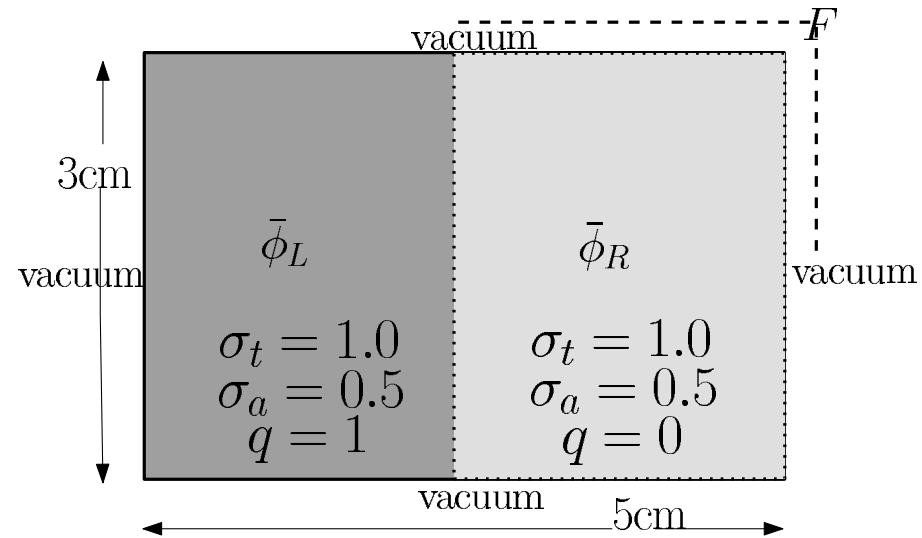


orthogonal grid

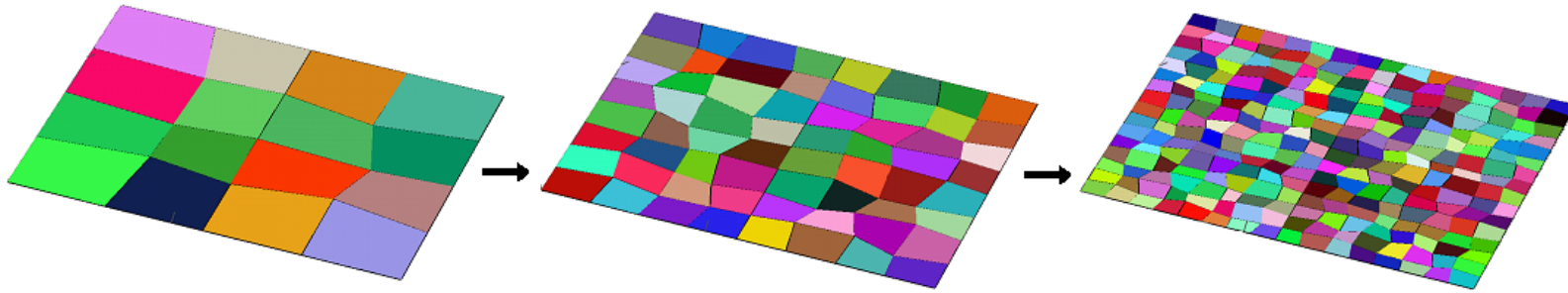


randomized (20%) grid

Transport Test Problem



Numerical Results



Results of Single Level Grids

	Orthogonal Grid			Randomized Grid			Relative Difference		
	F	ϕ_L	ϕ_R	F	ϕ_L	ϕ_R	F	ϕ_L	ϕ_R
8 × 8	2.998e-2	1.1217	0.1467	2.872e-2	1.1263	0.1435	4.2e-2	-4.0e-3	2.2e-2
16 × 16	3.141e-2	1.1021	0.1564	3.124e-2	1.1045	0.1543	5.4e-3	-2.2e-3	1.4e-2
32 × 32	3.194e-2	1.0975	0.1589	3.205e-2	1.0977	0.1581	-3.4e-3	-2.4e-4	5.0e-3
64 × 64	3.209e-2	1.0965	0.1593	3.216e-2	1.0964	0.1592	-2.2e-3	1.2e-4	8.4e-4

Numerically Estimated Spatial Order of Convergence

	Orthogonal Grid			Randomized Grid		
	F	ϕ_L	ϕ_R	F	ϕ_L	ϕ_R
single-level	1.82	2.32	2.66	2.88	2.35	1.86
two-level (with refinement on the left)	1.50	1.95	1.94	2.07	1.53	1.42
two-level (with refinement on the right)	1.40	2.23	2.35	1.29	1.86	1.89

Nonlinear Weighted Flux (NWF) Methods

- The transport (high-order) equation

$$\vec{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, \vec{\Omega}) + \sigma_t(\vec{r}) \psi(\vec{r}, \vec{\Omega}) = \frac{1}{4\pi} \sigma_s(\vec{r}) \phi(\vec{r}) + \frac{1}{4\pi} q(\vec{r}).$$

- The factors

$$G_m(\vec{r}) = \Gamma_m \int_{\omega_m} w(\Omega_x, \Omega_y) \psi(\vec{r}, \vec{\Omega}) d\vec{\Omega} \bigg/ \int_{\omega_m} \psi(\vec{r}, \vec{\Omega}) d\vec{\Omega}, \quad \Gamma_m = \frac{\int_{\omega_m} d\vec{\Omega}}{\int_{\omega_m} w(\Omega_x, \Omega_y) d\vec{\Omega}}.$$

$$F_m^\alpha(\vec{r}) = \Gamma_m \int_{\omega_m} |\Omega_\alpha| w(\Omega_x, \Omega_y) \psi(\vec{r}, \vec{\Omega}) d\vec{\Omega} \bigg/ \int_{\omega_m} \psi(\vec{r}, \vec{\Omega}) d\vec{\Omega}, \quad \alpha = x, y,$$

- The low-order NWF equations $\phi_m(\vec{r}) = \int_{\omega_m} \psi(\vec{r}, \vec{\Omega}) d\vec{\Omega}$, $m = 1, \dots, 4$

$$\nu_m^x \frac{\partial}{\partial x} (F_m^x \phi_m) + \nu_m^y \frac{\partial}{\partial y} (F_m^y \phi_m) + \sigma_t G_m \phi_m = \frac{1}{4} (\sigma_s \phi + q), \quad \phi = \sum_{m=1}^4 \phi_m .,$$

$$\nu_1^x = \nu_1^y = 1, \quad \nu_2^x = -1, \quad \nu_2^y = 1, \quad \nu_3^x = \nu_3^y = -1, \quad \nu_4^x = 1, \quad \nu_4^y = -1,$$

Asymptotic Diffusion Limit of the Transport Equation

- We define a small parameter ε , scaled cross sections and source:

$$\sigma_t = \frac{\hat{\sigma}_t}{\varepsilon}, \quad \sigma_a = \varepsilon \hat{\sigma}_a, \quad q = \varepsilon \hat{q},$$

- Consider that $\varepsilon \rightarrow 0$.
- We now assume that the solution can be expanded in power series of ε

$$\psi = \sum_{n=0}^{\infty} \varepsilon^n \psi^{[n]},$$

- The leading-order solution of the transport equation meets to the diffusion equation

$$-\frac{\partial}{\partial x} \frac{1}{3\sigma_t} \frac{\partial \psi^{[0]}}{\partial x} - \frac{\partial}{\partial y} \frac{1}{3\sigma_t} \frac{\partial \psi^{[0]}}{\partial y} + \sigma_a \psi^{[0]} = q.$$

Asymptotic Diffusion Limit of the Low-Order NWF Equations

- We consider various weights
 - $w(\Omega_x, \Omega_y) = 1$
 - $w(\Omega_x, \Omega_y) = |\Omega_x| + |\Omega_y|$
 - $w(\Omega_x, \Omega_y) = 1 + |\Omega_x| + |\Omega_y|$
 - $w(\Omega_x, \Omega_y) = 1 + \beta(|\Omega_x| + |\Omega_y|)$

Values of the diffusion coefficients (D) for specific NWF methods

Weight	1	$ \Omega_x + \Omega_y $	$1 + \Omega_x + \Omega_y $	$1 + \beta(\Omega_x + \Omega_y)$
D	$\frac{1}{4\sigma_t}$	$\left(\frac{\pi+2}{3\pi}\right)^2 \frac{1}{\sigma_t} \approx \frac{1}{3.36\sigma_t}$	$\left(\frac{4+5\pi}{12\pi}\right)^2 \frac{1}{\sigma_t} \approx \frac{1}{3.66\sigma_t}$	$\frac{1}{3\sigma_t}$

Numerical Results

- Test problem
 - A unit square domain
 - $\sigma_t = \frac{1}{\epsilon}$, $\sigma_a = \epsilon$, and $q = \epsilon$
 - $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$, and 10^{-5}
 - Boundary conditions are vacuum.
 - A uniform spatial mesh consists of 19×19 equal cells.
 - The compatible product quadruple-range quadrature set uses 3 polar and 3 azimuthal angles per octant.

Relative errors of the cell-average scalar flux in the cell located at the center

ϵ	Weight			
	1	$ \Omega_x + \Omega_y $	$1 + \Omega_x + \Omega_y $	$1 + \beta(\Omega_x + \Omega_y)$
10^{-2}	2.56E-1	1.01E-1	1.75E-1	7.13E-3
10^{-3}	2.68E-1	9.82E-2	1.79E-1	-2.18E-3
10^{-4}	2.69E-1	9.86E-2	1.80E-1	-1.99E-3
10^{-5}	2.69E-1	9.86E-2	1.80E-1	-1.97E-3

Asymptotic Boundary Condition

- There exist a boundary layer with the width of order of ε .
- The scalar flux at the boundary of the diffusive domain

$$\phi^{[0]}(X, y) = 2 \int_{\vec{n} \cdot \vec{\Omega} < 0} W(|\vec{n} \cdot \vec{\Omega}|) \psi_{in}(X, y, \vec{\Omega}) d\vec{\Omega},$$

- It is possible to improve the performance of the NWF method by using

$$w(\Omega_x, \Omega_y) = 1 + \lambda(|\Omega_x| + |\Omega_y|) + \kappa|\Omega_x\Omega_y|$$

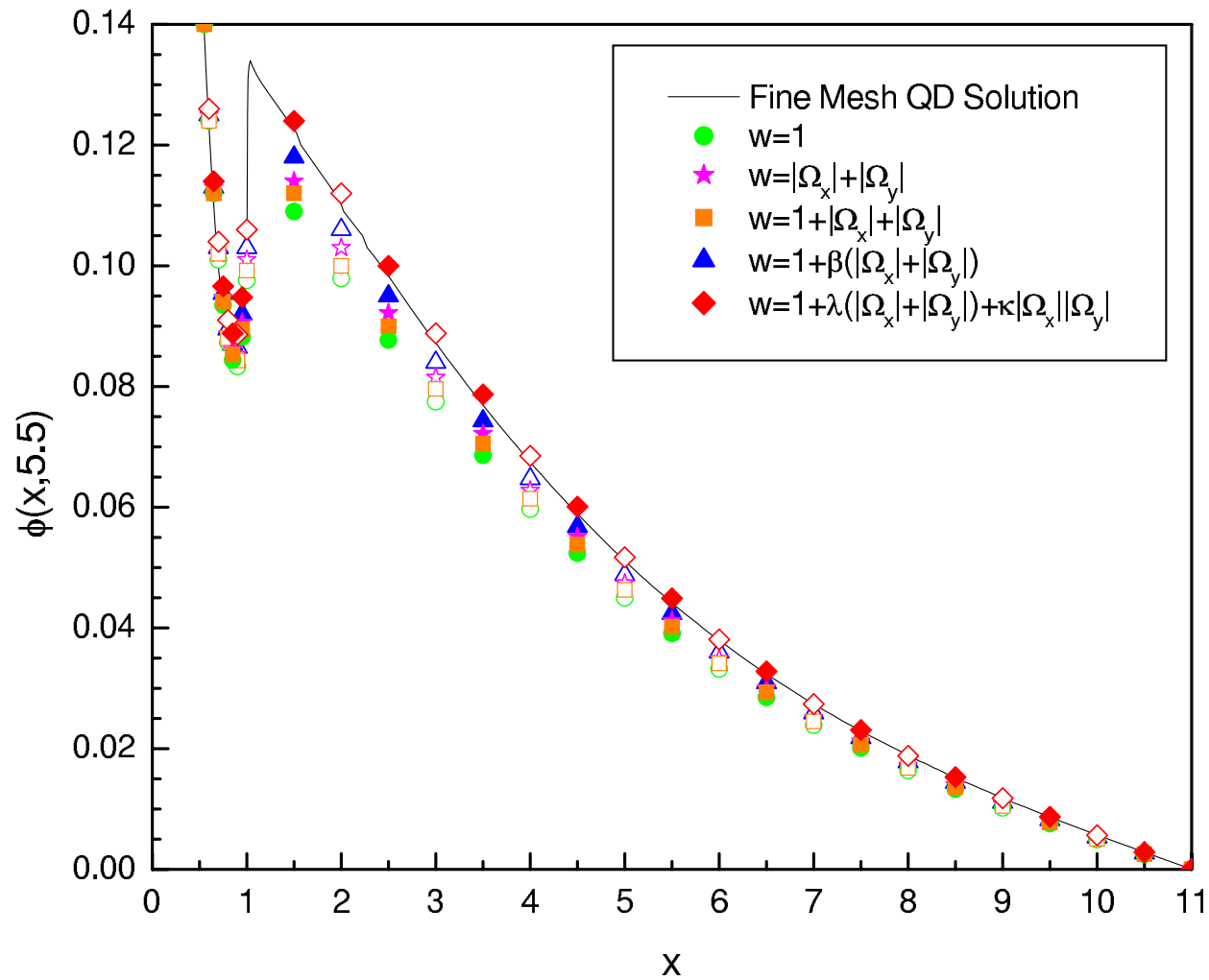
Relative errors of the asymptotic boundary conditions for the NWF methods

τ (mfp)	BLD Transport Method	Weight				
		1	$ \Omega_x + \Omega_y $	$1 + \Omega_x + \Omega_y $	w_β	$w_{\lambda, \kappa}$
0.0	0.033 %	0.033%	0.033%	0.033%	0.033%	-0.059%
0.2	-0.112%	-3.451%	-1.456%	-2.410%	-0.249%	-0.199%
1.0	-0.304%	-8.035%	-4.030%	-5.945%	-1.607%	0.697%
2.0	-0.423%	-10.871%	-6.557%	-8.620%	-3.948%	1.36%
4.0	-0.568%	-14.339%	-10.850%	-12.518%	-8.739%	1.25%
6.0	-0.641%	-16.089%	-13.520%	-14.748%	-11.97%	0.755%

Problem with an Unresolved Boundary Layer

- A domain $0 \leq x, y \leq 11$ with two subregions:
 1. $0 \leq x \leq 1$, $\sigma_t = 2$, $\sigma_s = 0$, $q = 0$, $\Delta x = 0.1$, and $\Delta y = 1$,
 2. $1 \leq x \leq 11$, $\sigma_t = \sigma_s = 100$, $q = 0$, and $\Delta x = \Delta y = 1$.
- There is an isotropic incoming angular flux with magnitude $\frac{1}{2\pi}$ on the left boundary
- Other boundary condition are vacuum.
- This problem enables one to test the ability of a method to reproduce an accurate diffusion solution in the interior of the diffusive region with the spatially unresolved boundary layer.

Problem with an Unresolved Boundary Layer



Conclusions

- We have developed a new method for solving the LOQD equations on arbitrary quadrilateral and AMR-like grids
 - The resulting QD method for solving transport problems demonstrated good performance on both randomized and AMR-like grids.
 - Observe second order spatial convergence in numerical tests
- We defined a new parameterized family of nonlinear flux methods for solving the 2D transport equation.
 - The asymptotic diffusion analysis enabled us to find a particular method of this family the solution of which satisfies a good approximation of the diffusion equation in diffusive regions.
 - As a result, we developed a 2D flux method with an important feature for solving transport problems with optically thick regions.
 - Note that it is possible to formulate a linear version of the proposed methods.