High Order Finite Volume Nonlinear Schemes for the Boltzmann Transport Equation

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AGENDA

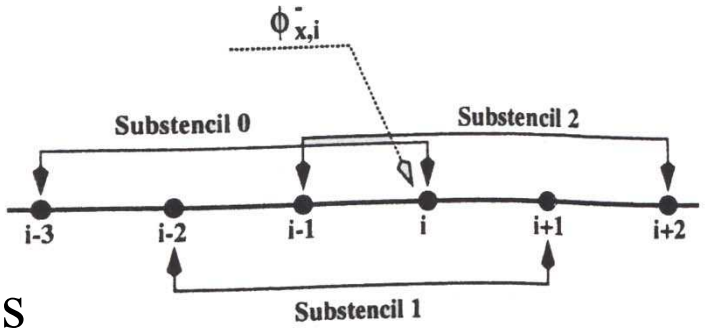
- Brief introduction to the *essentially nonoscillatory* family of schemes
- Finite volume (FV) WENO schemes
- FV WENO for the Boltzmann Transport Equation
- Numerical results (1-D, 2-D, 3-D):

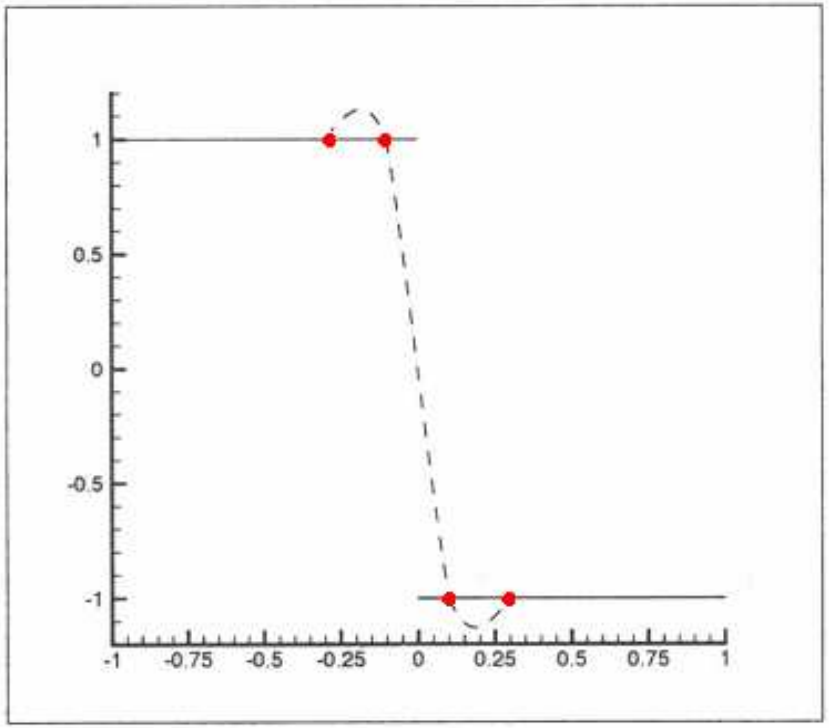
INTRODUCTION – ENO

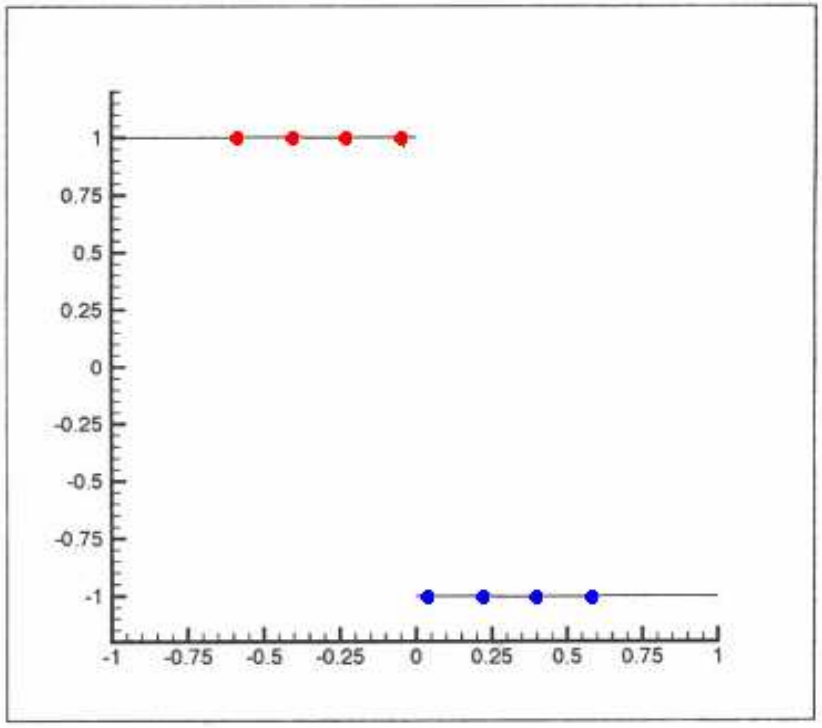
- Motivation: generalize Harten's very successful TVD scheme (1983) to higher than second-order accuracy.
- Original UNO/ENO papers by Harten and Osher, followed by Harten, Engquist, Osher and Chakravarthy, both published in 1987.
- Non-linear scheme (even for linear PDE's)
- Originally developed for *finite volume* schemes
- In essence, it is an *interpolation technique*.
- ENO scheme design principles:
  1. uniformly high order reconstruction (interpolation)
  2. conservation
  3. stencil avoids discontinuities/sharp gradients
- ENO evaluates several stencils, and chooses one of them: the one with "smallest" derivatives
- Finite difference ENO introduced by Shu and Osher, in 1988.

ENO Method

- Polynomial of *n*-th order
- *(n+1)* possible stencils
  - the least oscillating is chosen
- WENO - weighting of the polynomials







INTRODUCTION (Cont.'d) – WENO

- WENO (Weighted essentially nonoscillatory) schemes came about in 1994, by Liu, Osher and Chan.
- First developed for finite volume schemes (like ENO).
- WENO (convexly) combines all stencils, with weights based on smoothness
- Advantages of WENO over ENO:
  - (i) Higher order in smooth regions ($2k-1$ for kth order ENO)
  - (ii) Smoother stencil transition
  - (iii) Higher efficiency on vector computers: No if-then-else statements
- WENO is also applicable to both finite difference and finite volume schemes.

INTRODUCTION (Cont.'d) – FD WENO

- Finite difference (FD) WENO first used by Jiang and Shu, in 1996.
- More efficient than FV WENO: it avoids the reconstruction step.
- FD only applicable to structured grids.
- FD WENO (and ENO) only applicable to Cartesian grids.
- In general, WENO is recommended for problems that:
  1 are unsteady
  2 contain steep gradients (strong shocks, contacts, reaction fronts, etc.) **and**
  3 rich, smooth structure (vortices, boundary layers, shear layers, etc.)

THE 3-D BOLTZMANN TRANSPORT EQUATION

- In its general form, it is a scalar initial boundary value problem (IBVP), more specifically, an integro-differential equation in ψ:

$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \Omega \cdot \nabla \psi + \sigma \psi = \int_0^\infty \int_{S^2} \psi \sigma_s d\Omega' dE' + q$$

where

$\psi = \psi(r, \Omega, E, t)$ is the particle flux
$r = (x, y, z) \in D = [a_x, b_x] \times [a_y, b_y] \times [a_z, b_z] \subset \mathbf{R}^3$
$\sigma = \sigma(r, E)$, the total cross section
$\Omega \in S^2$, the unit sphere in $\mathbf{R}^3$
$E \in (0, \infty), t \in (t_0, \infty)$, energy and time, respectively
$\sigma_s = \sigma_s(r, \Omega' \cdot \Omega, E' \to E)$, the scattering cross section
$q = q(r, \Omega, E, t)$ is an external source term
$v = v(E)$ is the particle speed

- subject to intial conditions

$$\psi(r, \Omega, E, t_0) = \psi_0(r, \Omega, E) \quad \text{at time} \quad t = t_0$$

and Dirichlet or reflecting boundary conditions (BC) on ∂D.

- Including the temporal variable, phase-space is 7-D.

THE 1-D BTE

- To illustrate derivation of the finite volume method, we simplify the 3-D BTE by assuming:

(1) one spatial dimension only: x ("slab geometry")
(2) it follows from (1) that Ω also has one component: μ
(3) a single energy group E ("mono-energetic")
(4) isotropic scattering: $\sigma_s = \frac{\sigma_0}{2}$

$$\frac{\partial \psi}{\partial t} + \mu \frac{\partial \psi}{\partial x} + \sigma \psi = \frac{\sigma_0}{2} \int_{-1}^{1} \psi d\mu' + q$$

where

$$0 \leq x \leq 1, -1 \leq \mu \leq 1, t \geq 0$$

subject to intial conditions

$$\psi(x, \mu, 0) = \psi_0(x, \mu) \quad \text{at time} \quad t = 0$$

and Dirichlet BC at $x = 0, 1$:

$$\psi(0, \mu, t) = g_0(\mu), \quad \text{for } \mu > 0$$

$$\psi(1, \mu, t) = g_1(\mu), \quad \text{for } \mu < 0$$

- We now have a total of 3 phase-space variables.

SEMI-DISCRETIZATION: SPACE AND DIRECTION

- The spatial grid is defined by "nodes" at $M+1$ half-indices

$$0 = x_{\frac{1}{2}} < \ldots < x_{m-\frac{1}{2}} < x_{m+\frac{1}{2}} < x_{M+\frac{1}{2}} = 1$$

- and "cells" (or "zones") for each integral index m, which is of size:

$$\Delta x_m = x_{m+\frac{1}{2}} - x_{m-\frac{1}{2}}$$

- In direction μ, we use *discrete ordinates collocation* at J Gaussian quadrature points (J even):

$$-1 < \mu_1 < \ldots < \mu_{\frac{J}{2}} < 0 < \mu_{\frac{J}{2}+1} < \ldots < \mu_J < 1$$

  which are symmetric about the origin:

$$\mu_{J+1-j} = -\mu_j$$

- The integral on the right hand side is approximated by (for each x):

$$\int_{-1}^{1} \psi(x,\mu) d\mu \approx \sum_{j=1}^{J} w_j \psi(x,\mu_j)$$

SPATIAL AVERAGING ("CONSERVATION FORM")

- Integrate the 1-D BTE over cell m to obtain:

$$\frac{\partial \psi_{m,j}}{\partial t} + \frac{\mu_j}{\Delta x_m}(\psi_{m+\frac{1}{2},j} - \psi_{m-\frac{1}{2},j}) + \sigma_m \psi_{m,j}$$

$$= \frac{\sigma_{0m}}{2} \sum_{j'=1}^{J} w_{j'} \psi_{m,j'} + q_{m,j}$$

where

$$\psi_{m\pm\frac{1}{2},j} = \psi(x_{m\pm\frac{1}{2}}, \mu_j)$$

$$\psi_{m,j} = \frac{1}{\Delta x_m} \int_{x_{m-\frac{1}{2}}}^{x_{m+\frac{1}{2}}} \psi(x, \mu_j) dx$$

$$\sigma_m = \frac{1}{\Delta x_m} \int_{x_{m-\frac{1}{2}}}^{x_{m+\frac{1}{2}}} \sigma(x) dx$$

$$\sigma_{0m} = \frac{1}{\Delta x_m} \int_{x_{m-\frac{1}{2}}}^{x_{m+\frac{1}{2}}} \sigma_0(x) dx$$

$$q_{m,j} = \frac{1}{\Delta x_m} \int_{x_{m-\frac{1}{2}}}^{x_{m+\frac{1}{2}}} q(x, \mu_j) dx$$

- We use Dirichlet boundary conditions for simplicity:

$$\psi_{\frac{1}{2},j} = g_0(\mu_j), \mu > 0$$

$$\psi_{M+\frac{1}{2},j} = g_1(\mu_j), \mu < 0$$

SPATIAL INTERPOLATION

- Need to relate point values (at half indices) to cell averages (at integer indices).
- There are many ways to do this: central scheme, (simple average), corner balance, 1st order upwind, etc.
- For example, with 1st order upwind we have:

$$\psi_{m+\frac{1}{2},j} = \begin{cases} \psi_{m+1,j}, & \text{if } \mu_j \leq 0 \\ \psi_{m,j}, & \text{if } \mu_j > 0 \end{cases}$$

  - very dissipative
- With central we have:

$$\psi_{m+\frac{1}{2},j} = \frac{1}{2}(\psi_{m+1,j} + \psi_{m,j})$$

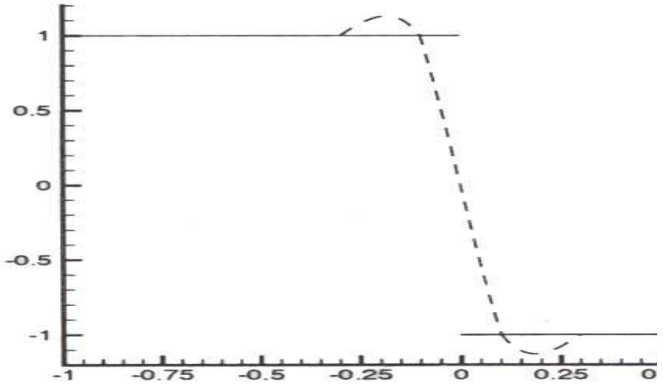
  - oscillatory (like Petrov-Galerkin node-centered)
- Higher order interpolations (i.e. reconstructions) of point values yield higher spatial accuracy.
- The higher the order of accuracy, the more important to control the oscillations
- Obvious choice: ENO or WENO interpolation

Advanced Methods

- Higher order polynomial used for reconstruction

⊕ higher accuracy

⊖ tendency to oscillations



➡ do not allow total variation to grow

FINITE VOLUME WENO IN SPACE

- For finite volume schemes the interpolation conditions must be treated as conditions on *cell averages* (ie. integrals) instead of simple point values.
- Up to second order, these two are the same.
- For WENO3 scheme we compute *three* **2nd order** polynomials, and use a linear combination of them.
- For the BTE, no flux splitting or expensive "Riemann solver" is necessary. (No characteristic decomposition necessary.)
- The scheme is fully conservative and the reconstruction is upwind (Riemann solver is trivial in this case).
- WENO3 Spatial discretization is only slightly more expensive than Petrov-Galerkin, and about the same as Corner Balance.
- Convergence to steady-state can be slower than other linear methods – need a good preconditioner.
- Fully parallelized with 2 (WENO3) or 3 (WENO5) ghost layers.
- Load balancing *not* affected by WENO.

WENO INTERPOLATION

- Given a *cell averaged* grid function $\{v_j\}_{j=1}^N$ on a set of grid cells $\{x_j\}$ corresponding to a grid $\{x_{j-\frac{1}{2}}\}$, we approximate $\bar{v}_{j+\frac{1}{2}}$ at the cell faces via a weighted linear combination of all possible interpolations:

$$v_{j+\frac{1}{2}} = \sum_{r=0}^{k-1} w_r v_{j+\frac{1}{2}}^{(r)}$$

  where typically $k = 2$ (for WENO3) or $k = 3$ (for WENO5).

- The $v_{j+\frac{1}{2}}^{(r)}$ are the various interpolated values using polynomials corresponding to stencil r.

- The weights are given by:

$$w_r = \frac{\alpha_r}{\sum_{s=0}^{k-1} \alpha_s}, \quad \text{for} \quad r = 0, ..., k-1$$

$$\alpha_r = \frac{d_r}{(\epsilon + \beta_r)^2}$$

WENO INTERPOLATION (Cont.'d)

- For the two most commonly used WENO schemes we have:
  if $k = 2$:

$$d_0 = \frac{2}{3}$$

$$d_1 = \frac{1}{3}$$

$$\beta_0 = (v_{i+1} - v_i)$$

$$\beta_1 = (v_i - v_{i-1})$$

  if $k = 3$:

$$d_0 = \frac{3}{10}$$

$$d_1 = \frac{3}{5}$$

$$d_2 = \frac{1}{10}$$

$$\beta_0 = \frac{13}{12}(v_i - 2v_{i+1} + v_{i+2})^2 + \frac{1}{4}(3v_i - 4v_{i+1} + v_{i+2})^2$$

$$\beta_1 = \frac{13}{12}(v_{i-1} - 2v_i + v_{i+1})^2 + \frac{1}{4}(v_{i-1} - v_{i+1})^2$$

$$\beta_2 = \frac{13}{12}(v_{i-2} - 2v_{i-1} + v_i)^2 + \frac{1}{4}(v_{i-2} - 4v_{i-1} + 3v_i)^2$$

WENO INTERPOLATION (Cont.'d)

- $\psi_{m+\frac{1}{2},j}$ is reconstructed in the upwind direction.
- Our formulation is general enough to be:
  (1) applicable on unequally spaced grids;
  (2) formally high order accurate for any grid (FV vs. FD);
  (3) "seamlessly" high order at processor boundaries and at reflecting boundaries via HYPRE ghost layers;
  (4) fully three dimensional.

OPERATOR (MATRIX) FORM

- The semidiscrete form can be written as a matrix operation on a solution vector $\mathbf{\Psi} = (\psi_{m,j})^T, 1 \leq m \leq M, 1 \leq j \leq J$:

$$\dot{\mathbf{\Psi}} + \mathbf{T}\mathbf{\Psi} - \mathbf{F} = 0$$

  where:
  $\dot{\mathbf{\Psi}} = \frac{\partial \mathbf{\Psi}}{\partial t}$ is the temporal derivative,
  $\mathbf{T}$ represents the semidiscrete operation in space and direction, and
  $\mathbf{F}$ includes source and boundary terms.

- In compact notation, we may write it as a system of ODE's (in general, with other types of BC's it becomes a differential- algebraic equation (DAE) system):

$$F(t, \mathbf{\Psi}, \dot{\mathbf{\Psi}}) = 0$$

- We have efficient time integrators that solve this in time (eg. IDA, PVODE).

1-D TEST PROBLEM, I

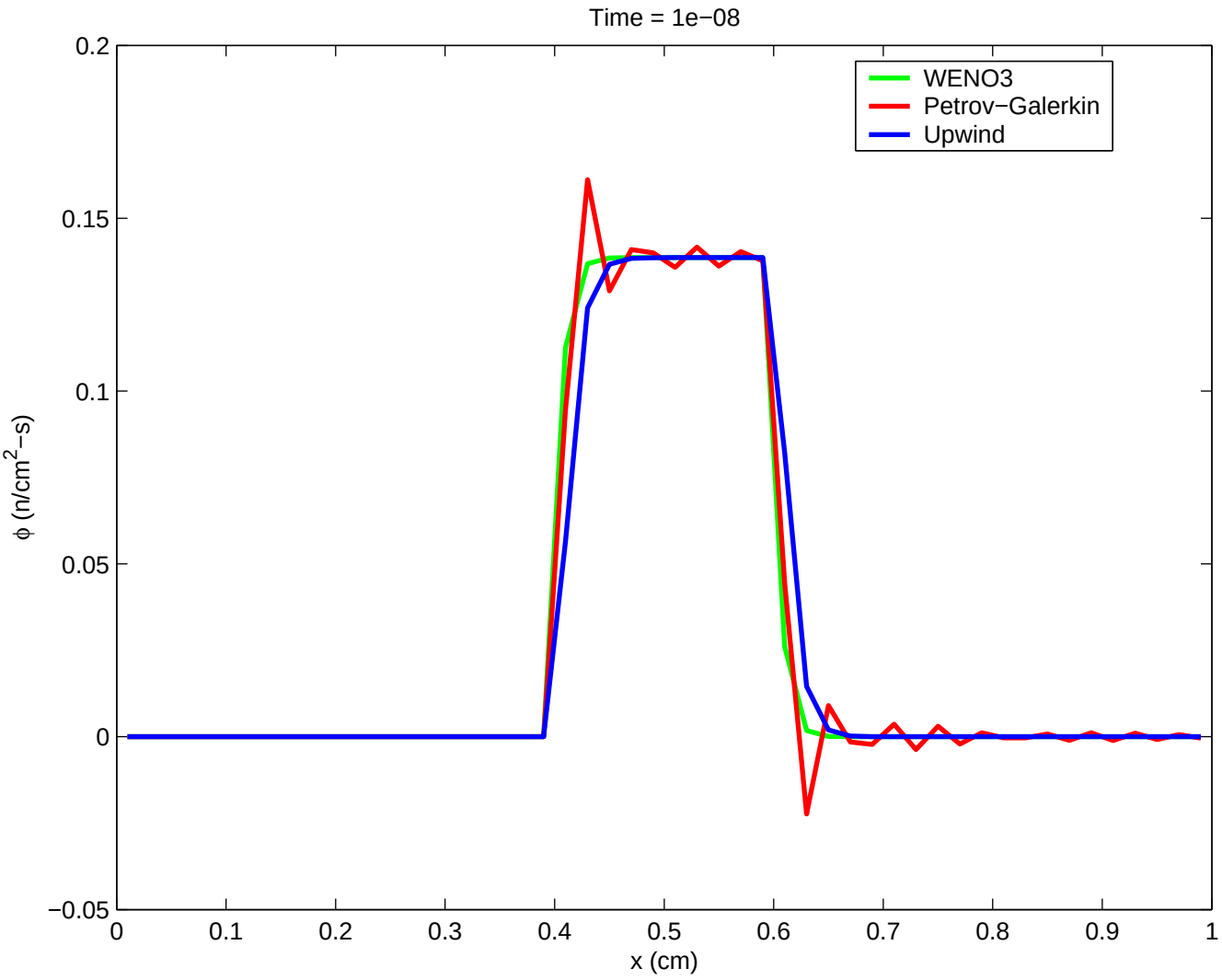
- IC: $\psi_0(x) = 0$ for $x \in [0, 1]$ at $t = 0$.
- Dirichlet BC at "inflow":

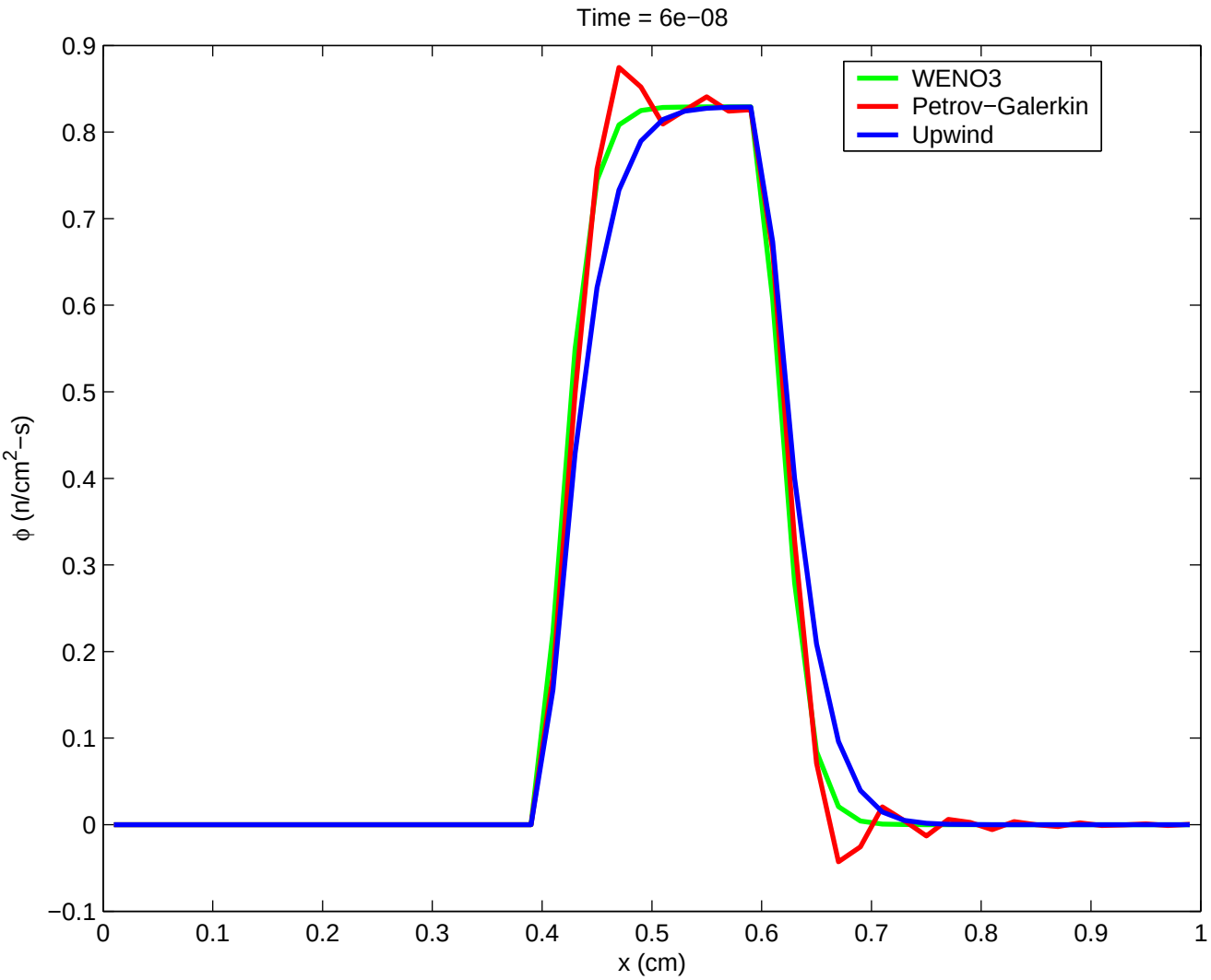
$$\psi(0, t) = 0 \quad \text{for} \quad \mu > 0$$

$$\psi(1, t) = 0 \quad \text{for} \quad \mu < 0$$

- $\sigma = 0.1$, $\sigma_s = 0.01$
- $$q = \begin{cases} 10, & \text{if } x \in [0.4, 0.6] \\ 0, & \text{otherwise} \end{cases}$$

- $N = 50$ grid cells
- Time-dependent simulation: used IDA for time integration.
- Compared WENO3 to:
  (i) Petrov-Galerkin finite element (node centered) scheme
  (ii) 1st order upwind scheme (node centered)


Time = 1e−08
WENO3
Petrov−Galerkin
Upwind
0.2
0.15
0.1
0.05
0
−0.05
ϕ (n/cm2−s)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)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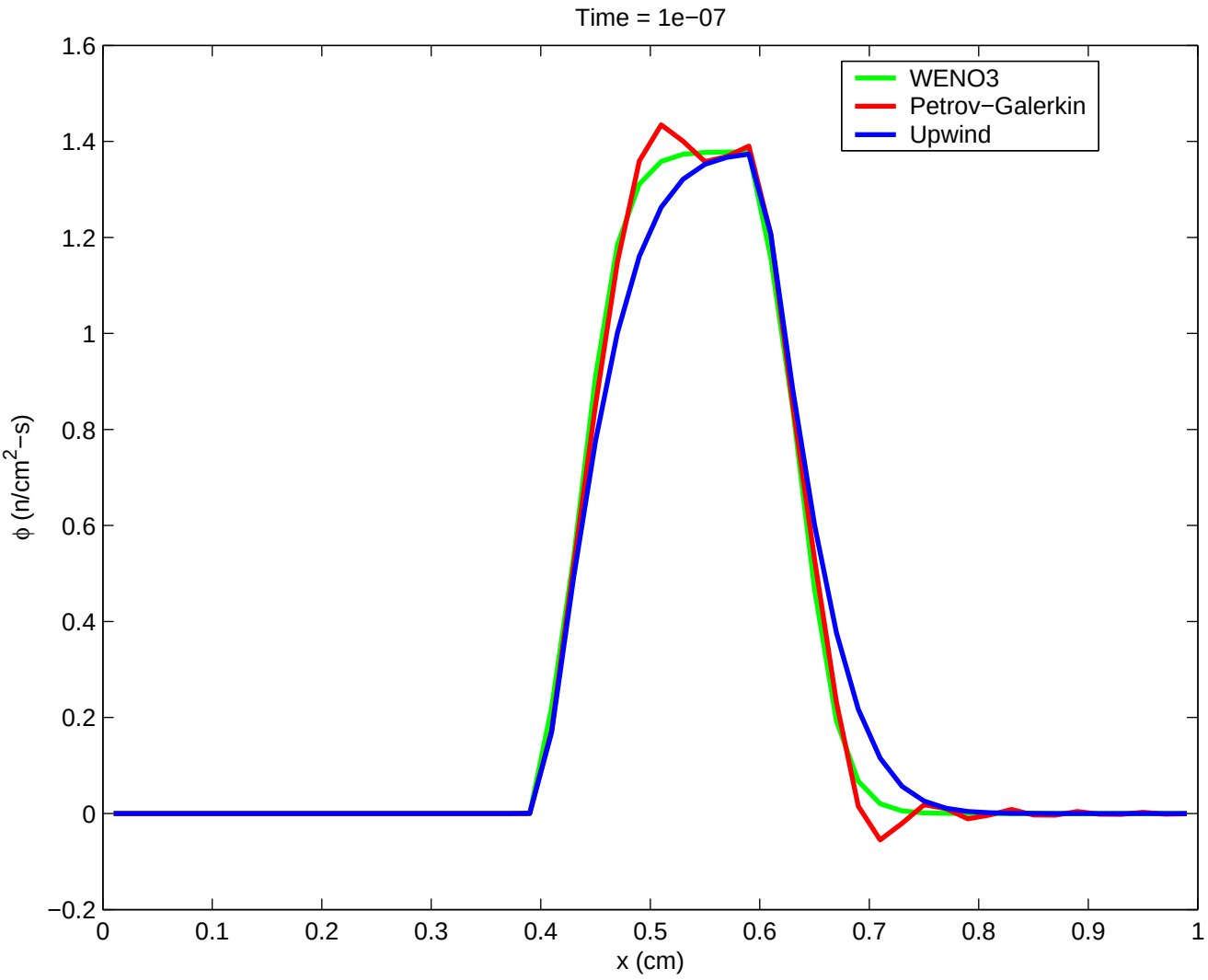
WENO3
Petrov−Galerkin
Upwind
ϕ (n/cm2−s)
x (cm)
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
−0.1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1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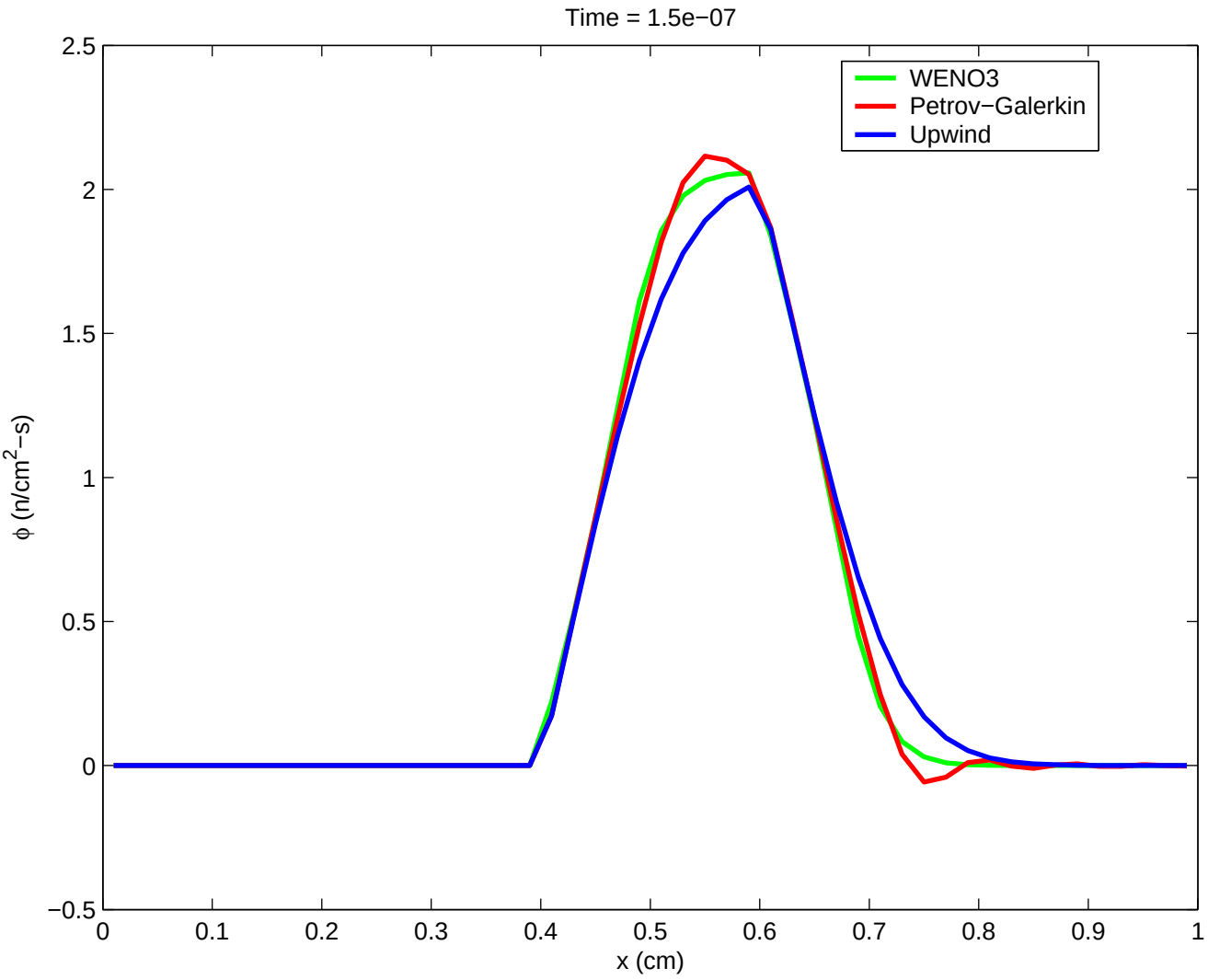
WENO3
Petrov−Galerkin
Upwind
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)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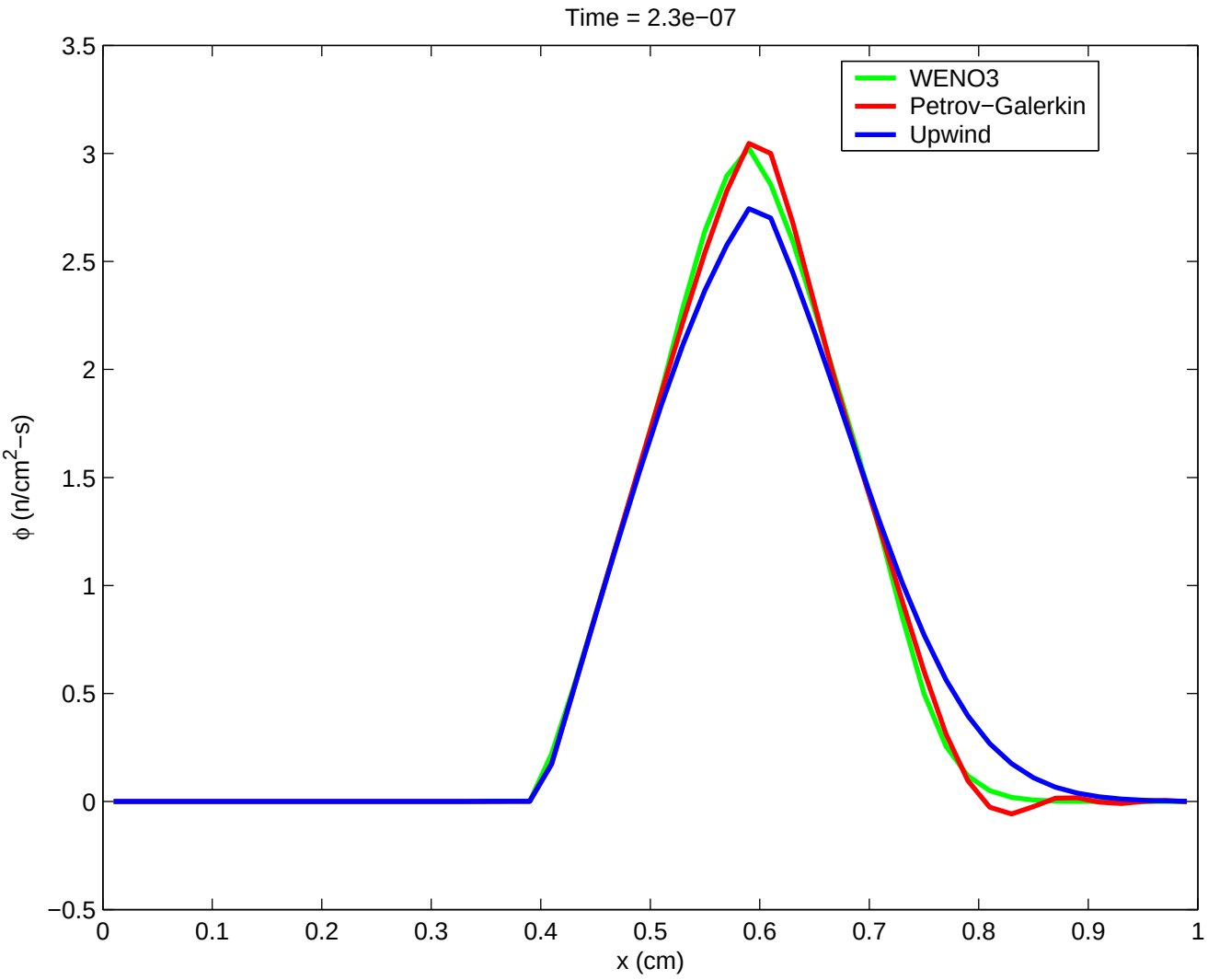
WENO3
Petrov−Galerkin
Upwind
2.5
2
1.5
1
0.5
0
−0.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)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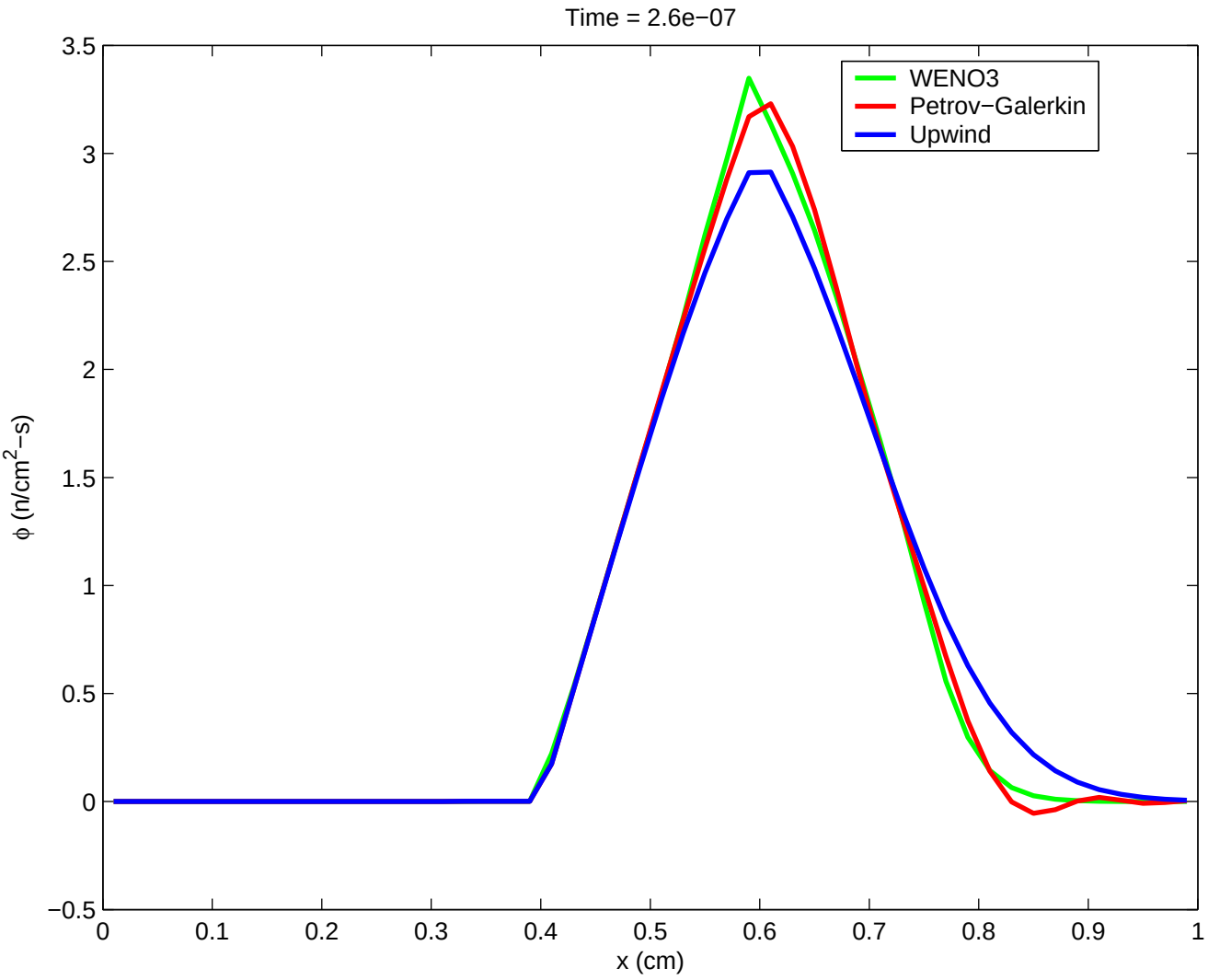
WENO3
Petrov−Galerkin
Upwind
3.5
3
2.5
2
1.5
1
0.5
0
−0.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)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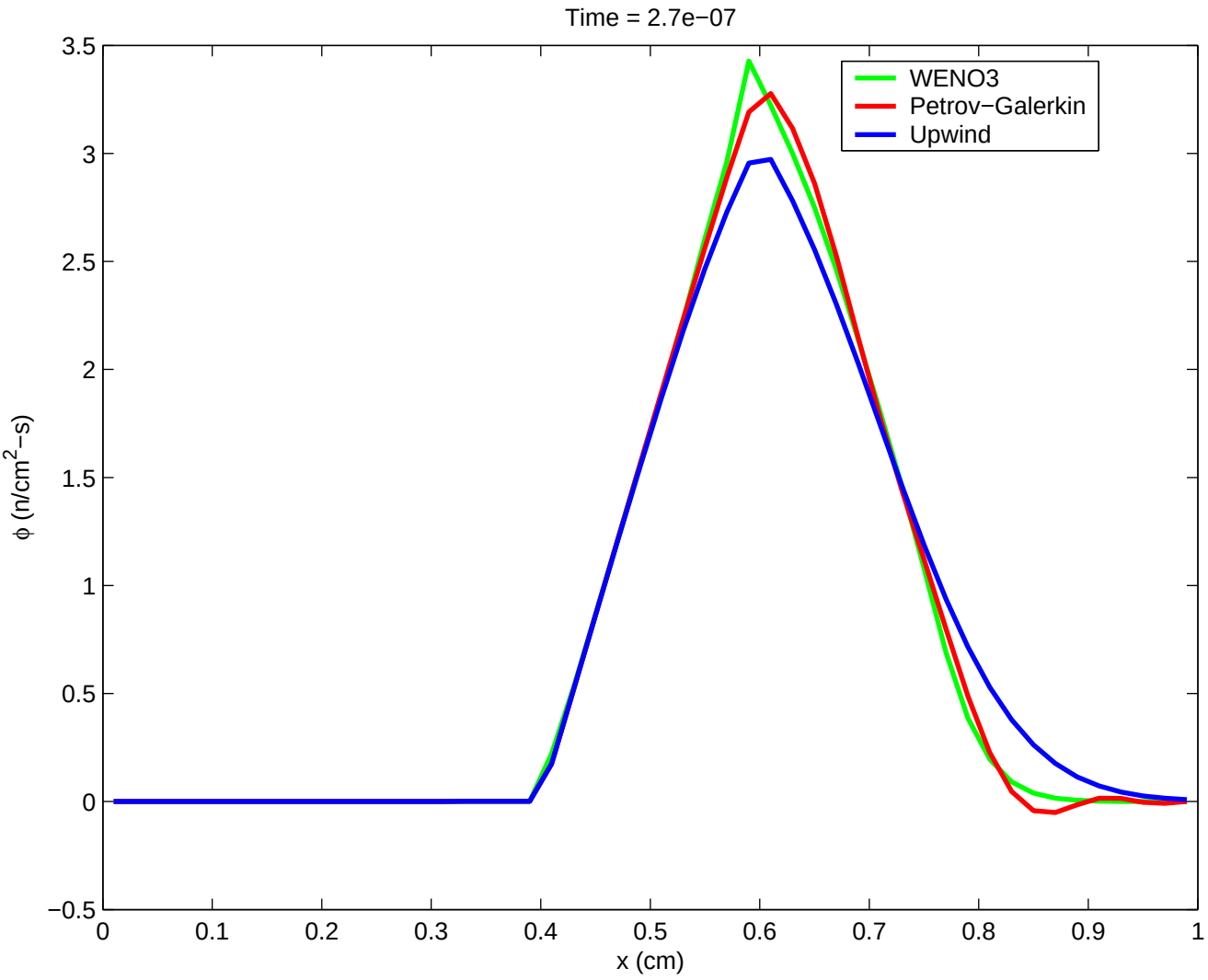
WENO3
Petrov−Galerkin
Upwind
3.5
3
2.5
2
1.5
1
0.5
0
−0.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)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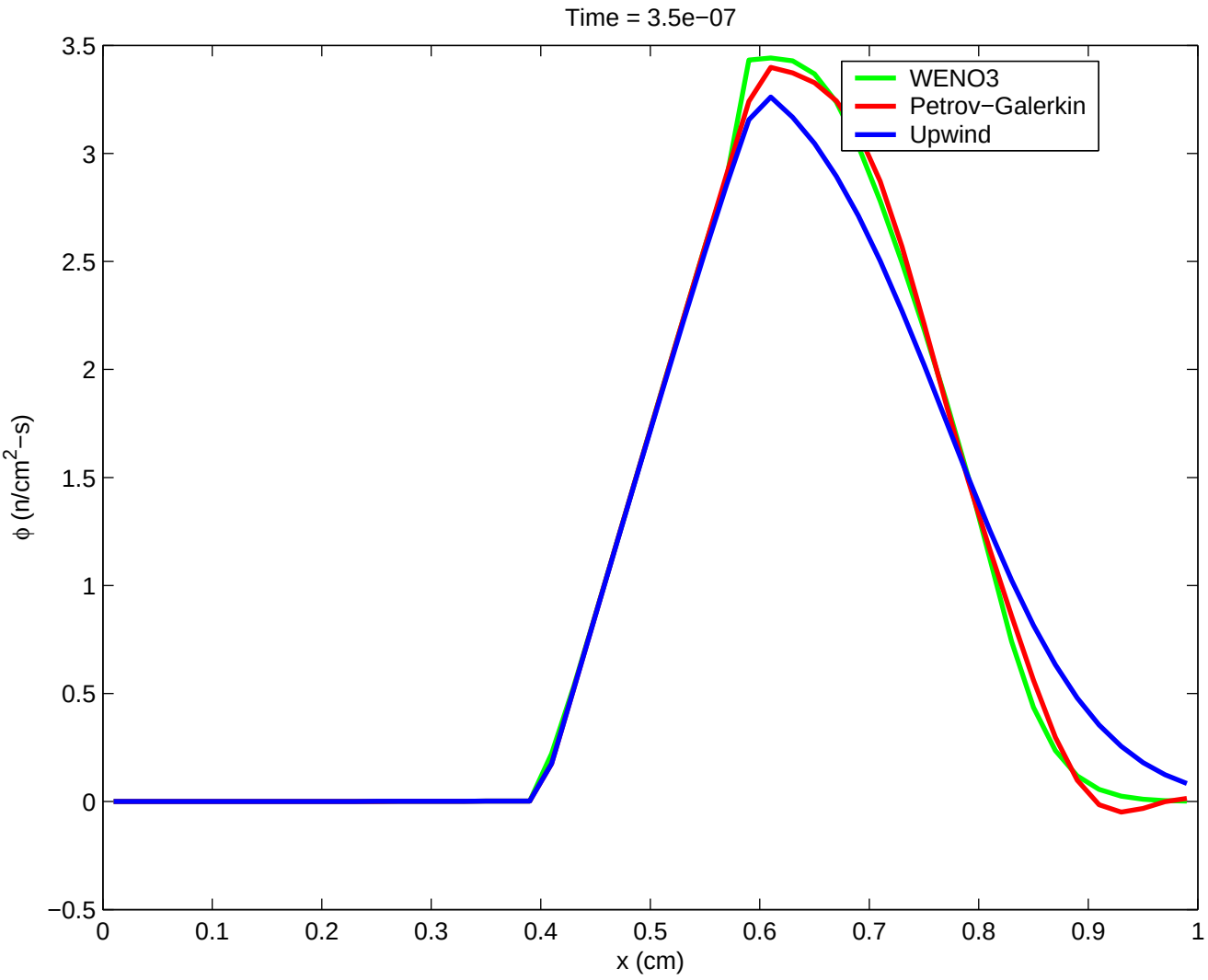
WENO3
Petrov−Galerkin
Upwind
3.5
3
2.5
2
1.5
1
0.5
0
−0.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)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Petrov−Galerkin
Upwind
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3
2.5
2
1.5
1
0.5
0
−0.5
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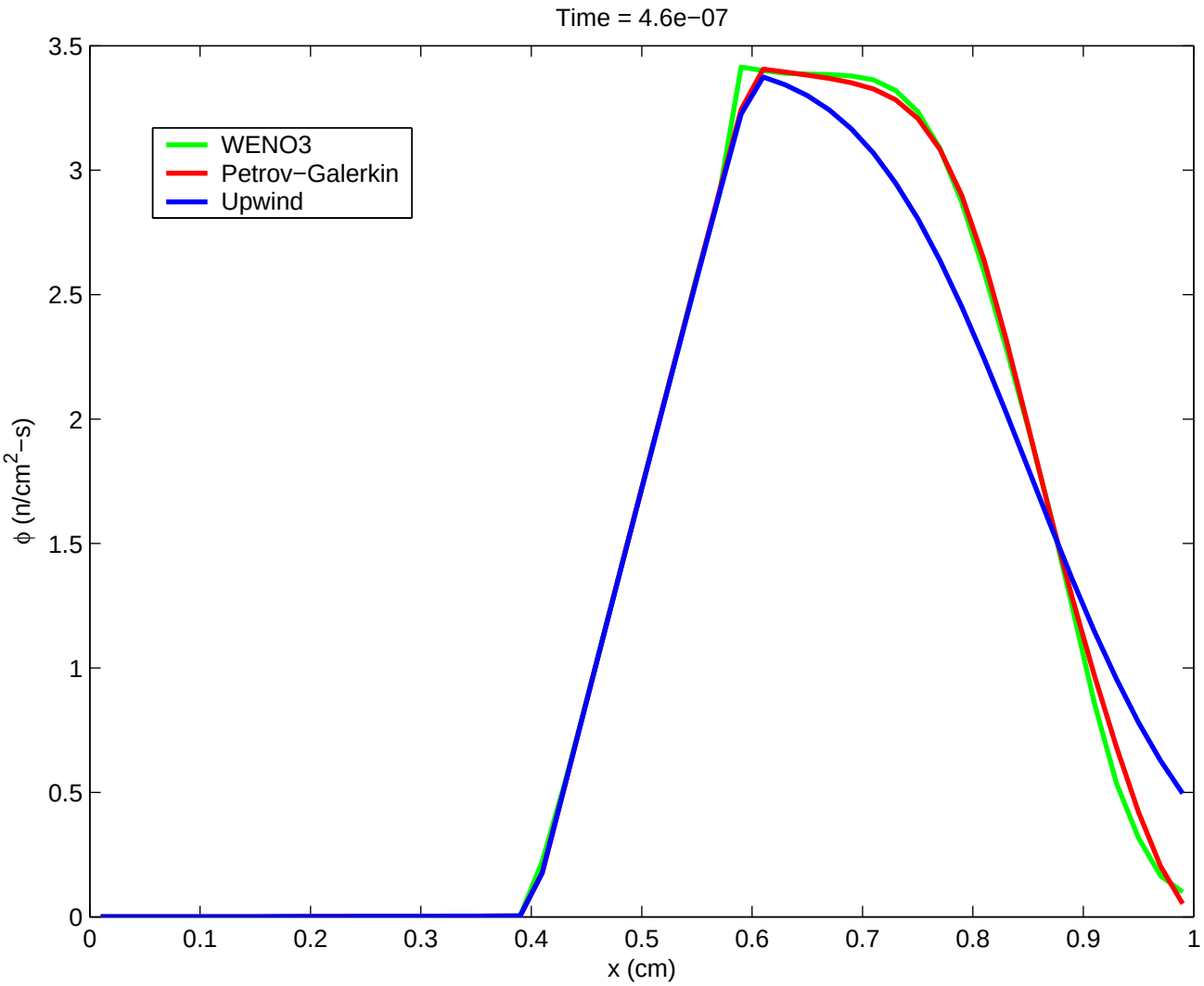
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)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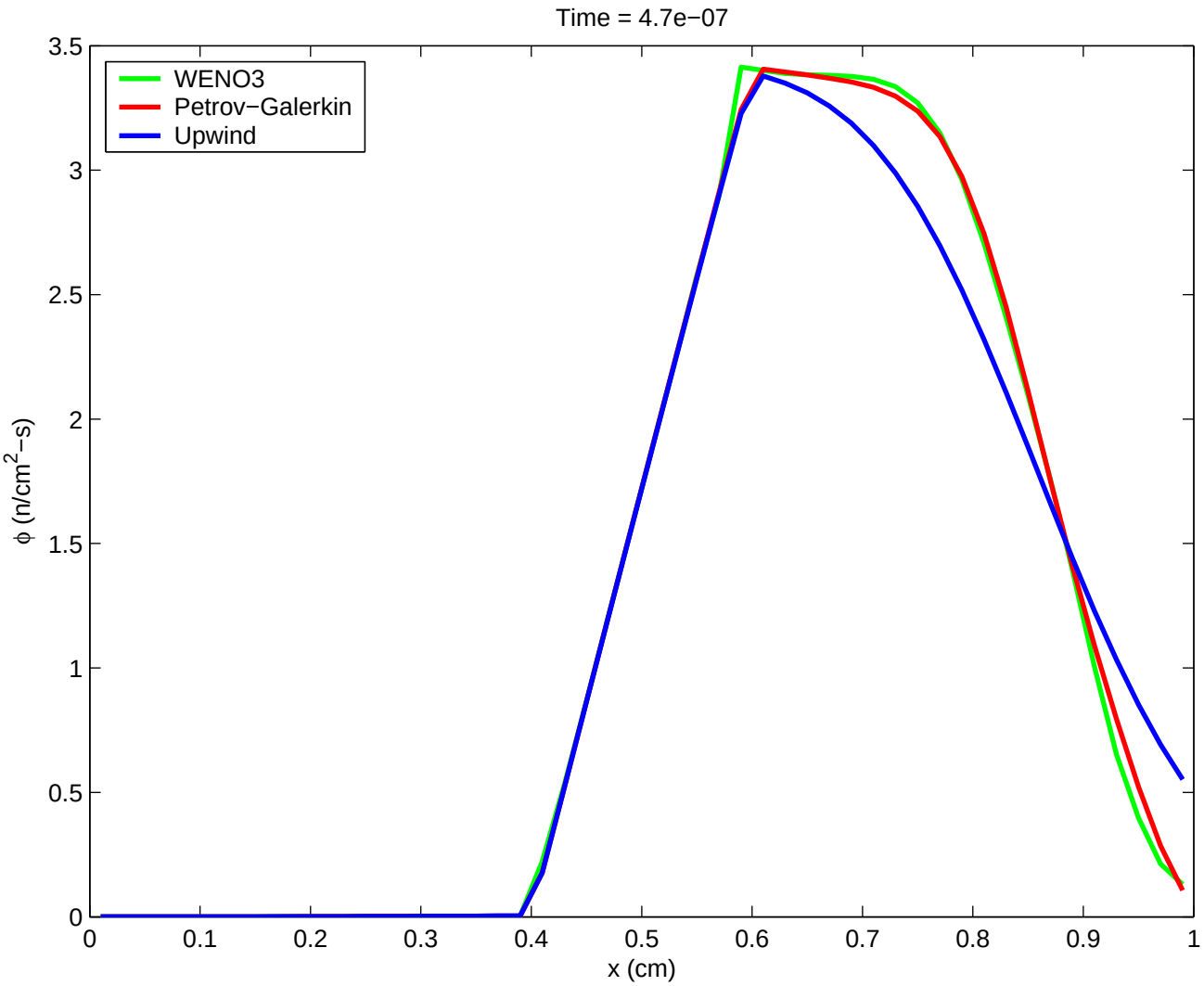
WENO3
Petrov−Galerkin
Upwind
φ (n/cm2−s)
x (cm)
0
0.5
1
1.5
2
2.5
3
3.5
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9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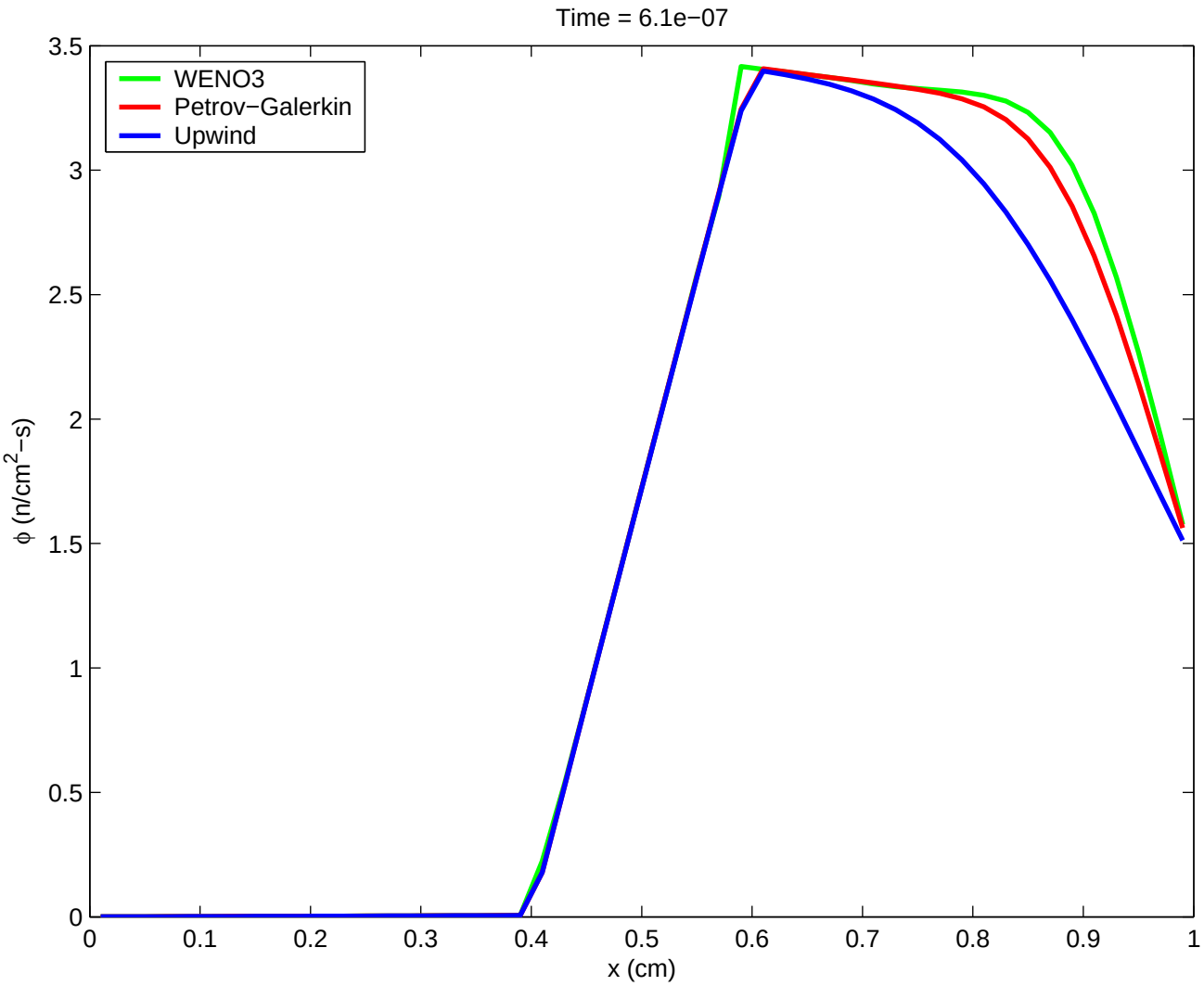
WENO3
Petrov−Galerkin
Upwind
3.5
3
2.5
2
1.5
1
0.5
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)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WENO3
Petrov−Galerkin
Upwind
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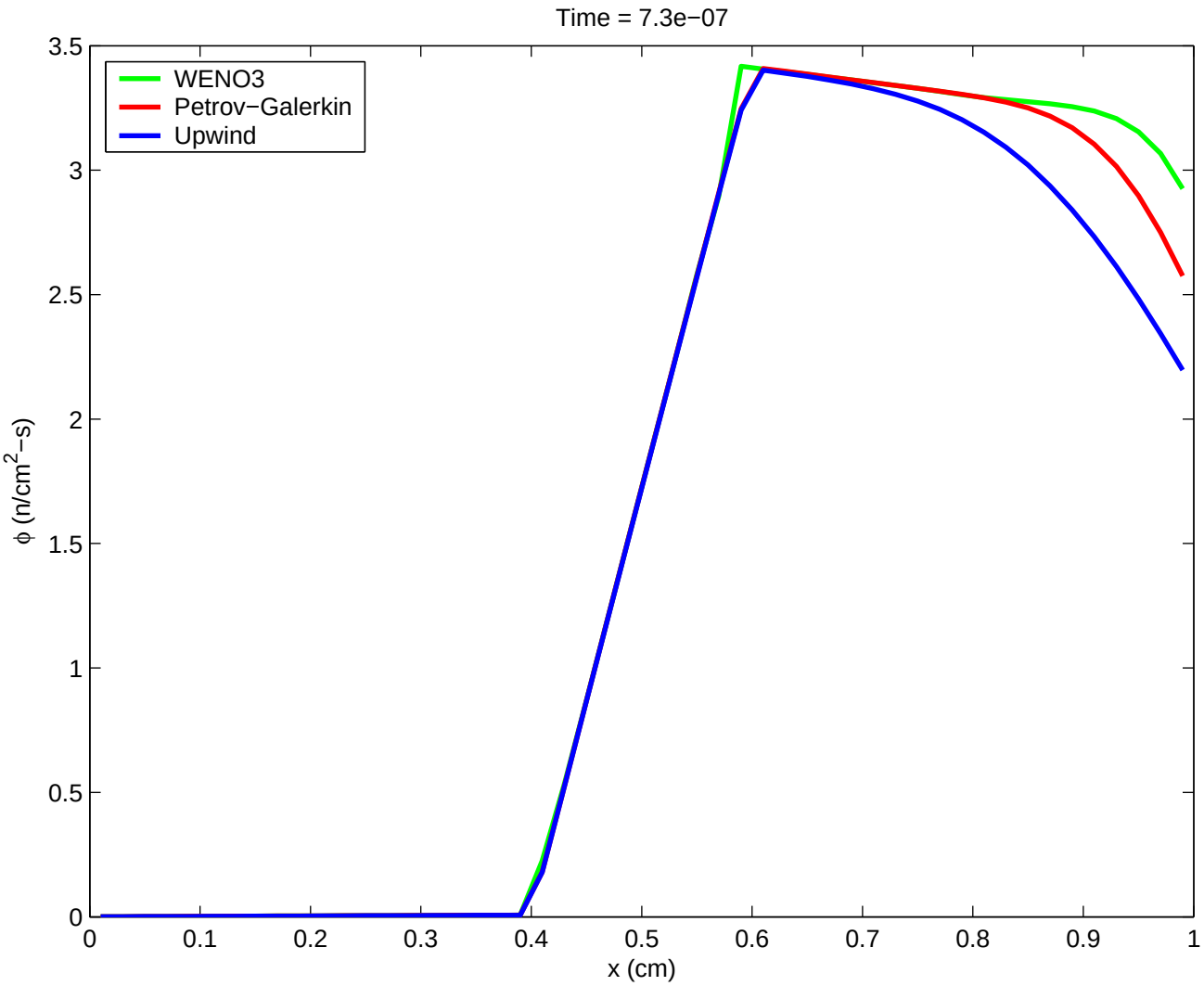
3
2.5
2
1.5
1
0.5
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)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WENO3
Petrov−Galerkin
Upwind
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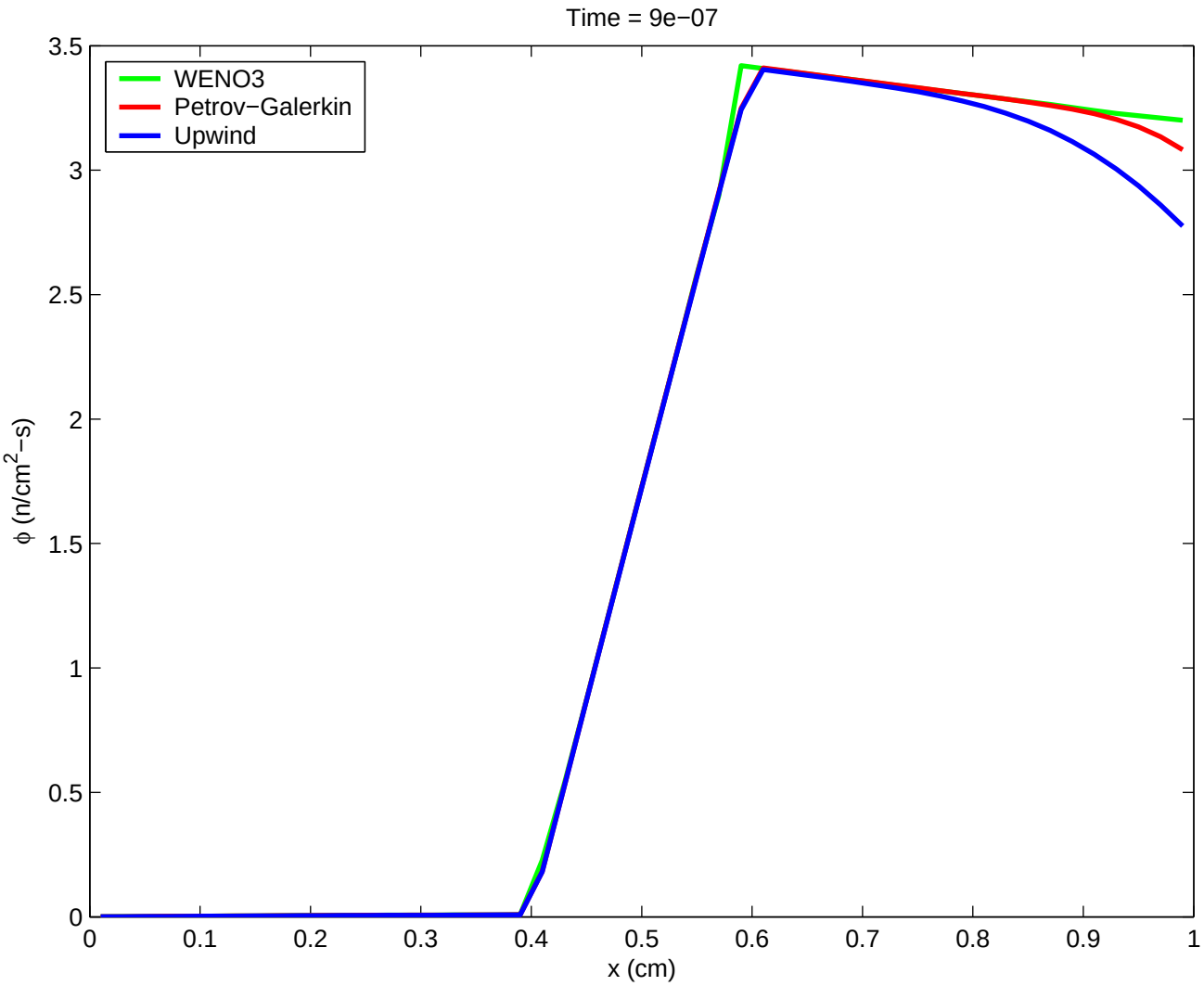
3
2.5
2
1.5
1
0.5
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)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WENO3
Petrov−Galerkin
Upwind
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2.5
2
1.5
1
0.5
0
0
0.1
0.2
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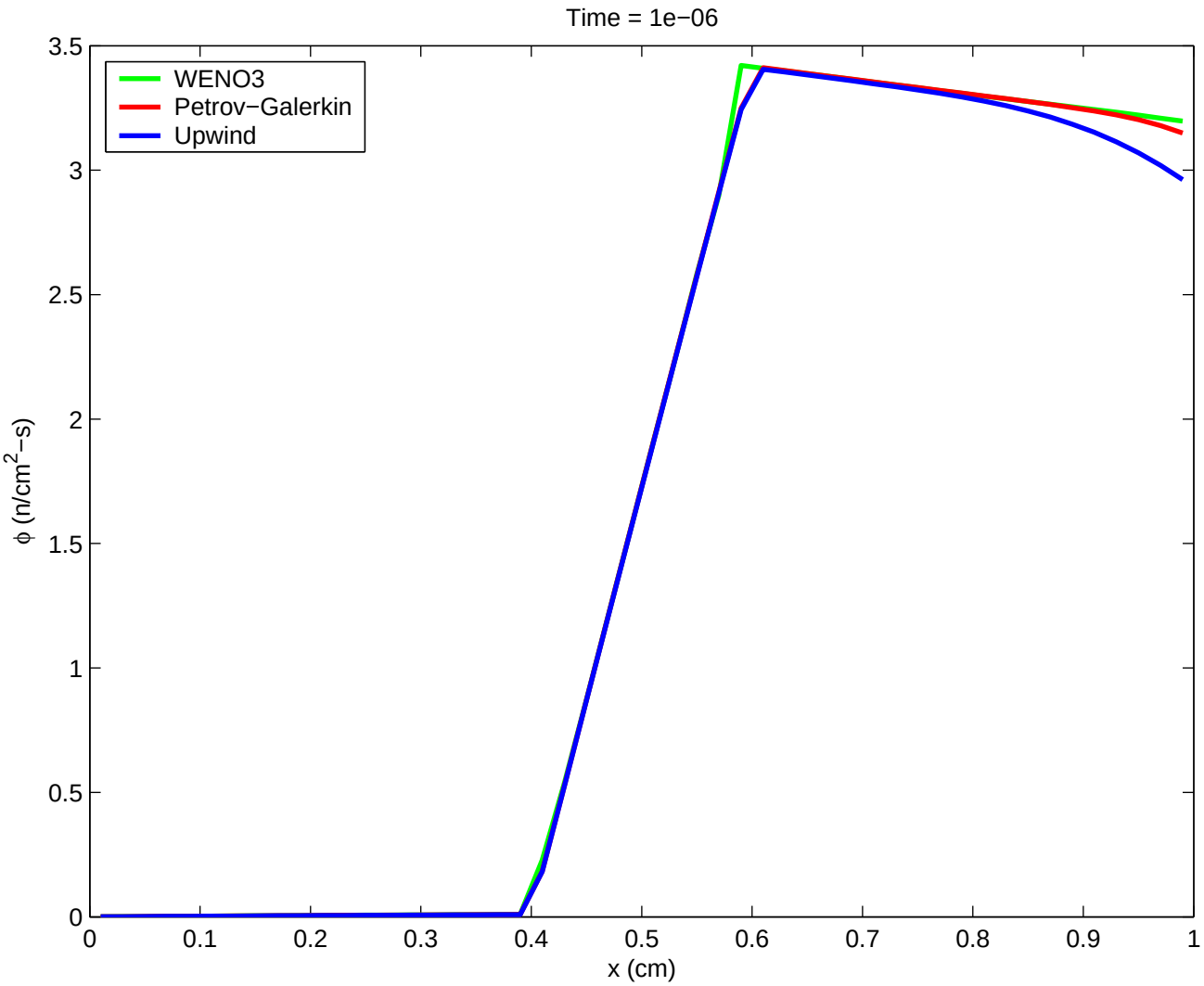
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)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Petrov−Galerkin
Upwind
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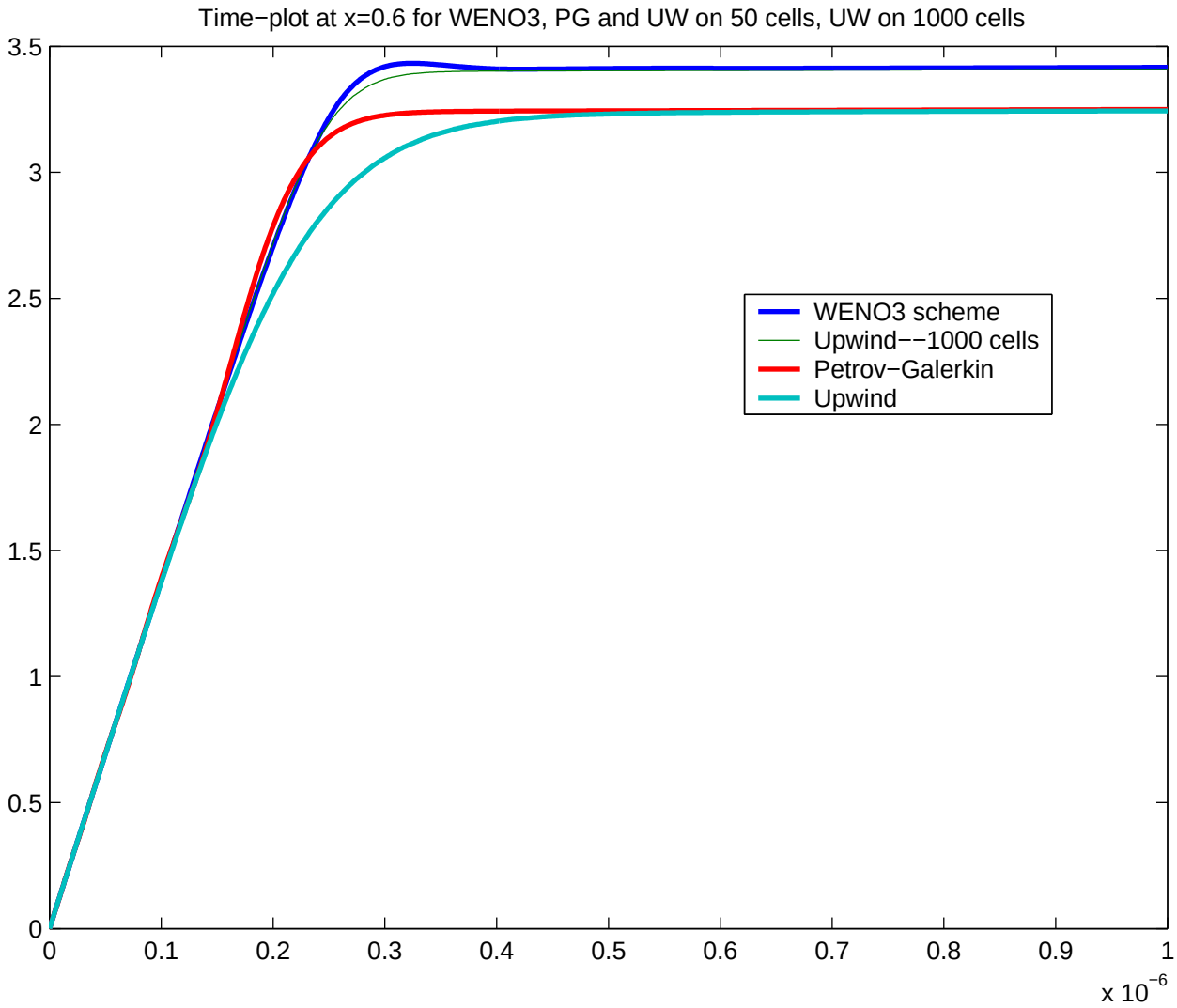
2.5
2
1.5
1
0.5
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)


Time−plot at x=0.6 for WENO3, PG and UW on 50 cells, UW on 1000 cells
3.5
3
2.5
2
1.5
1
0.5
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^−6
WENO3 scheme
Upwind−−1000 cells
Petrov−Galerkin
Upwind

1-D TEST PROBLEM, II

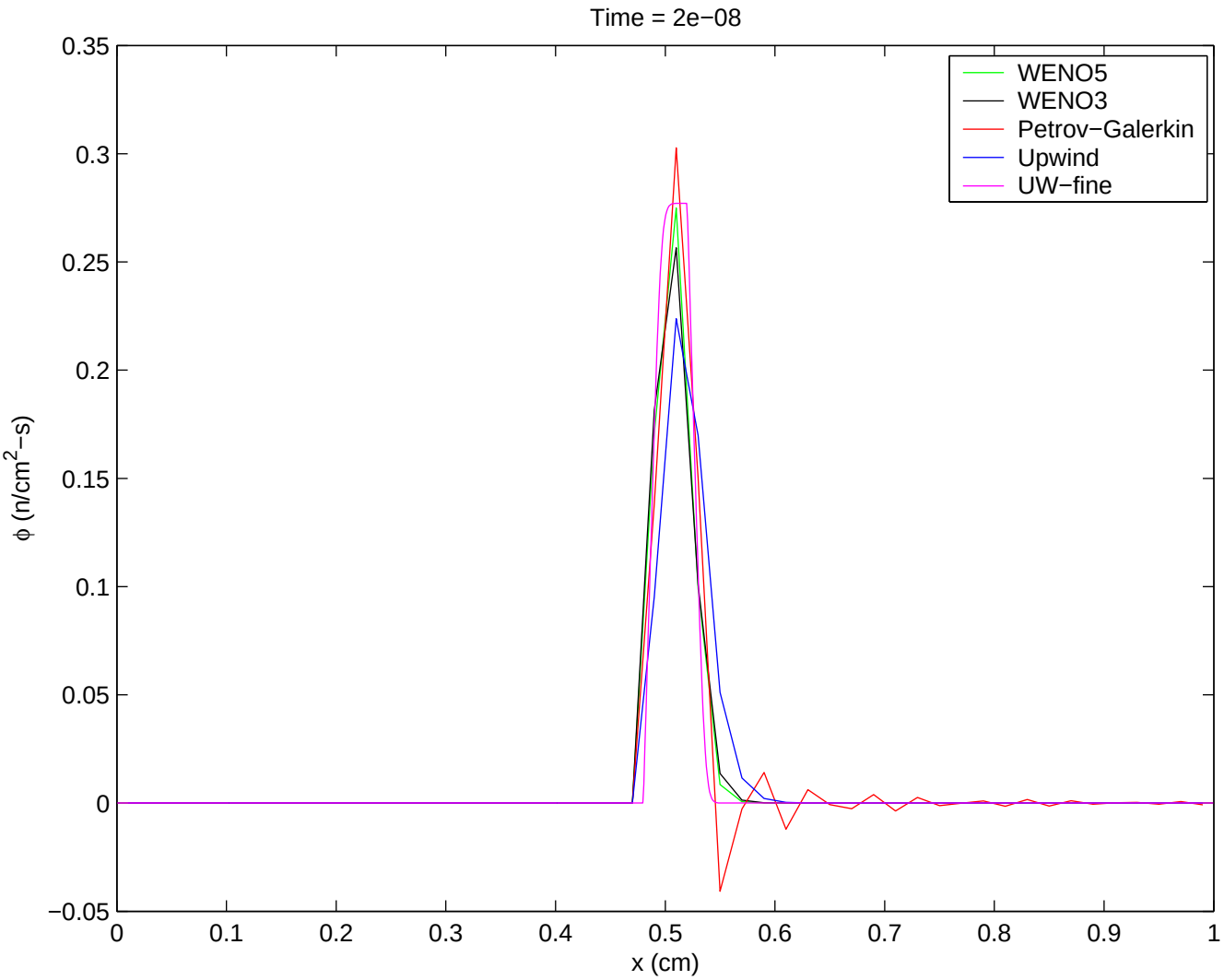
- IC: $\psi_0(x) = 0$ for $x \in [0, 1]$ at $t = 0$.
- Dirichlet BC at "inflow":

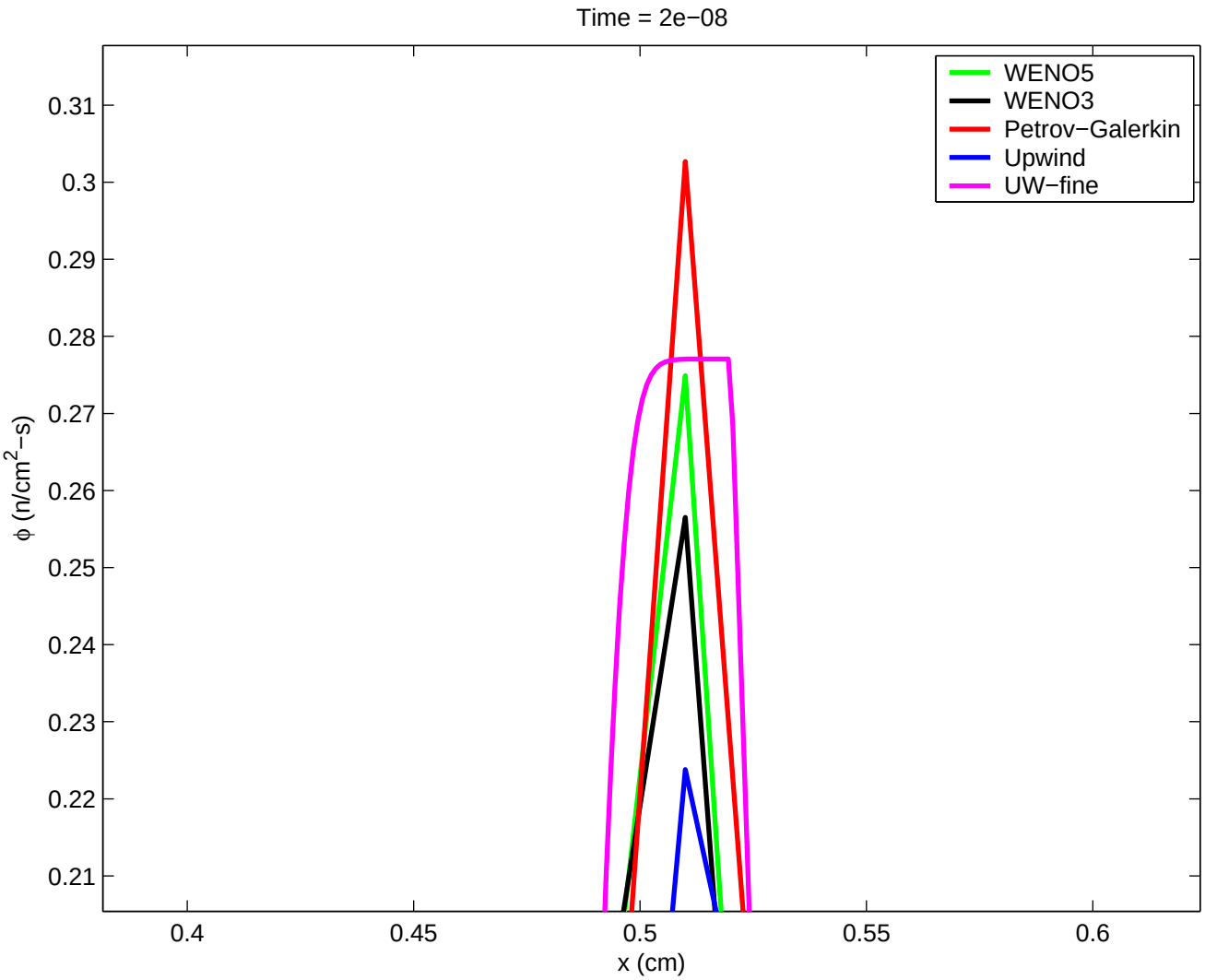
$$\psi(0, t) = 0 \quad \text{for} \quad \mu > 0$$

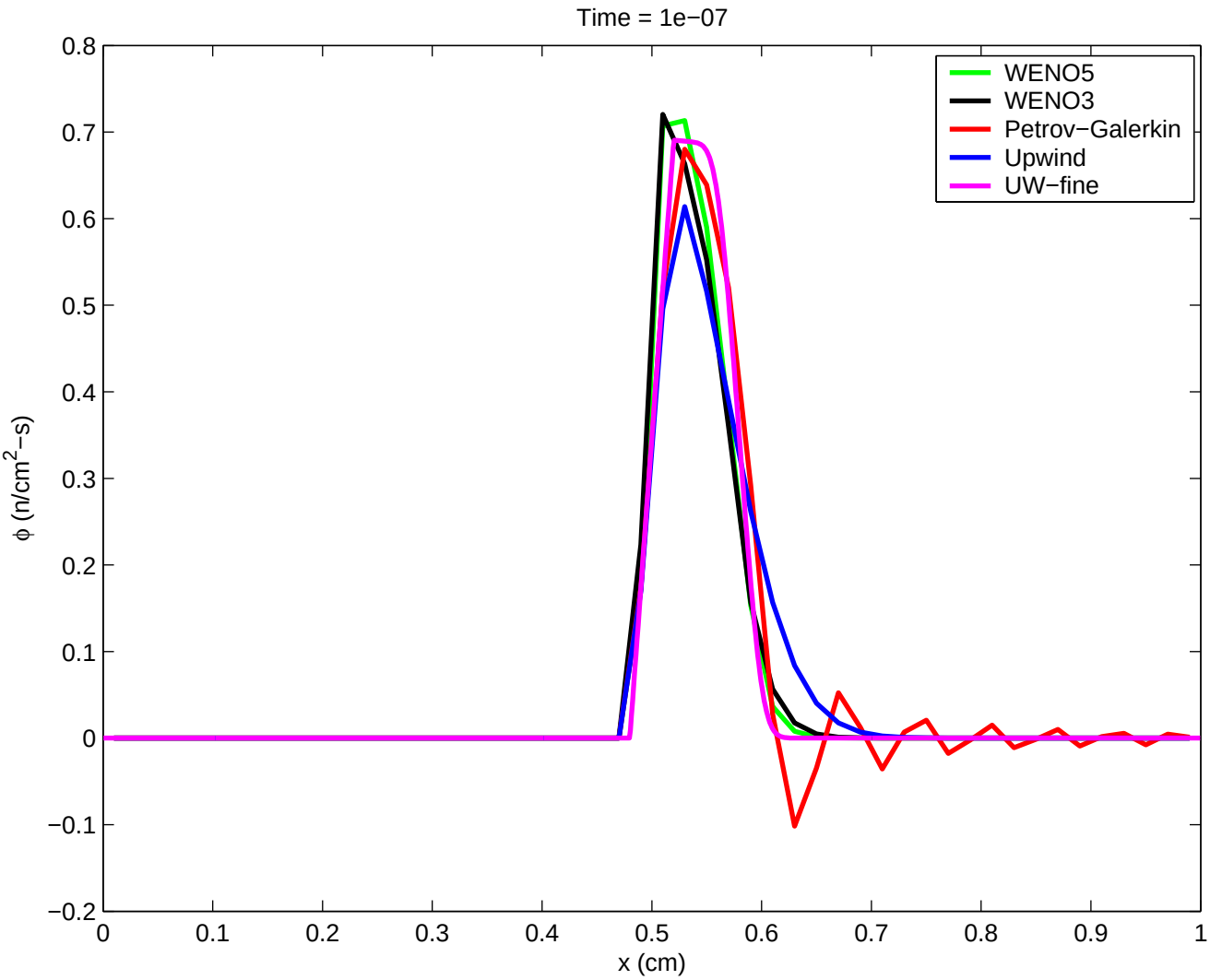
$$\psi(1, t) = 0 \quad \text{for} \quad \mu < 0$$

- $\sigma = 0.1$, $\sigma_s = 0.01$
- $$q = \begin{cases} 10, & \text{if } x \in [0.48, 0.52] \\ 0, & \text{otherwise} \end{cases}$$

- $N = 50$ grid cells
- Time-dependent simulation: used IDA for time integration.
- Compared WENO3 and WENO5 to:
  - (i) Petrov-Galerkin finite element (node centered) scheme
  - (ii) 1st order upwind scheme (node centered)
  - (iii) 1st order upwind on fine grid (1000 cells)

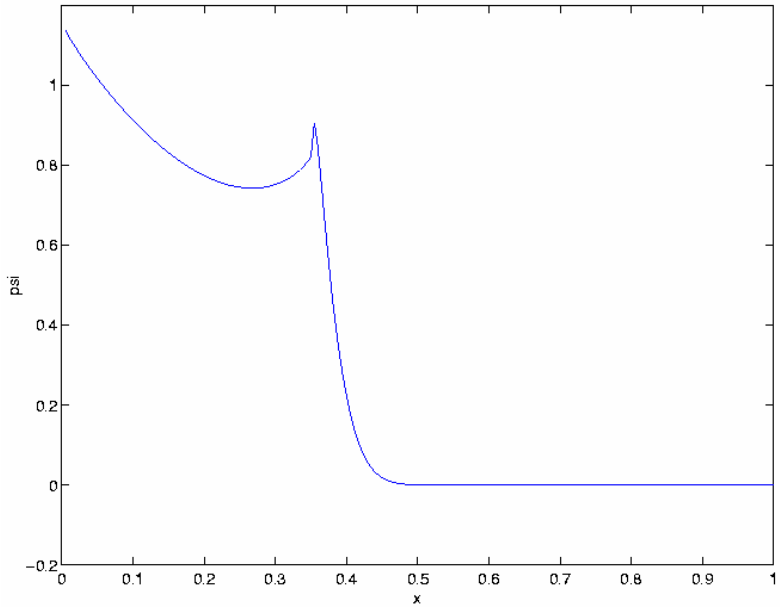

Time = 2e−08
WENO5
WENO3
Petrov−Galerkin
Upwind
UW−fine
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
−0.05
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)
ϕ (n/cm2−s)


Time = 2e−08
WENO5
WENO3
Petrov−Galerkin
Upwind
UW−fine
0.31
0.3
0.29
0.28
0.27
0.26
0.25
0.24
0.23
0.22
0.21
ϕ (n/cm2−s)
0.4
0.45
0.5
0.55
0.6
x (cm)

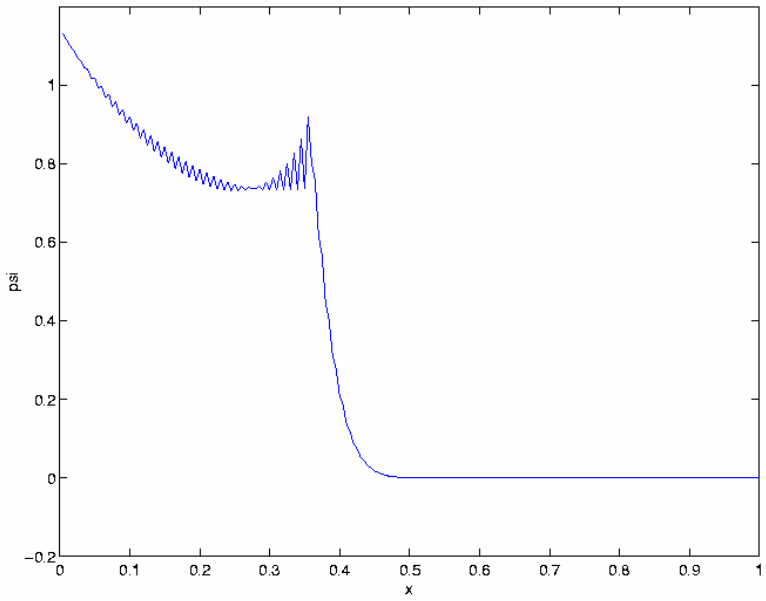

Time = 1e−07
WENO5
WENO3
Petrov−Galerkin
Upwind
UW−fine
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
−0.1
−0.2
ϕ (n/cm2−s)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x (cm)

Dirichlet boundary conditions of $\psi(0, t) = 1$,
$\sigma = 1$ for $x < 0.35$,
$\sigma = 100$ for $x > 0.35$, after time $t = 0.7$.

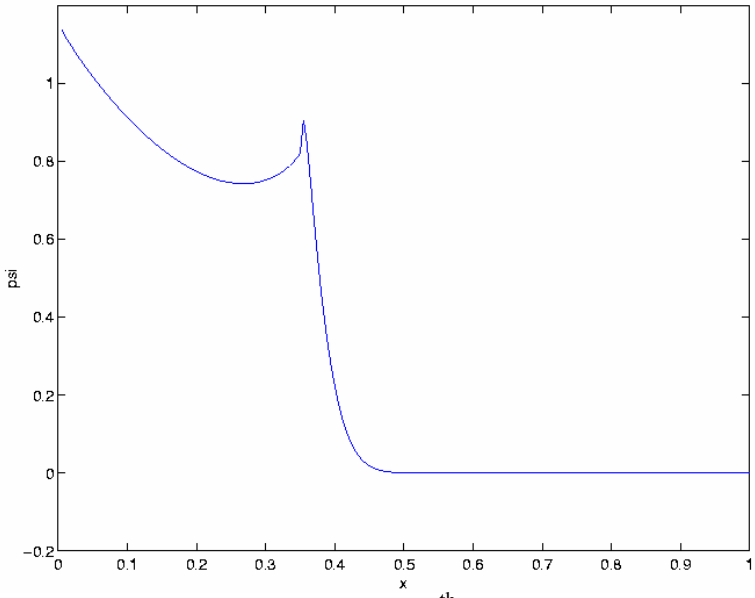
All results shown here are run with 200 spatial and 50 velocity discretization points, excepting the upwind model, which is run with 10,000 spatial and 50 velocity points. The output shown is a weighted sum of the spatial solutions at each velocity discretization point, representative of the solution that would be physically observed.



'Superfine' Upwind



Central Differencing



WENO – 5th order

2-D TEST PROBLEM

- IC: $\psi_0(x, y) = 0$ for $(x, y) \in [0, 100] \times [0, 100]$ at $t = 0$.
- Dirichlet BC at "inflow":

$$\psi(0, y, t) = 0 \quad \text{for} \quad \Omega_x > 0$$

$$\psi(100, y, t) = 0 \quad \text{for} \quad \Omega_x < 0$$

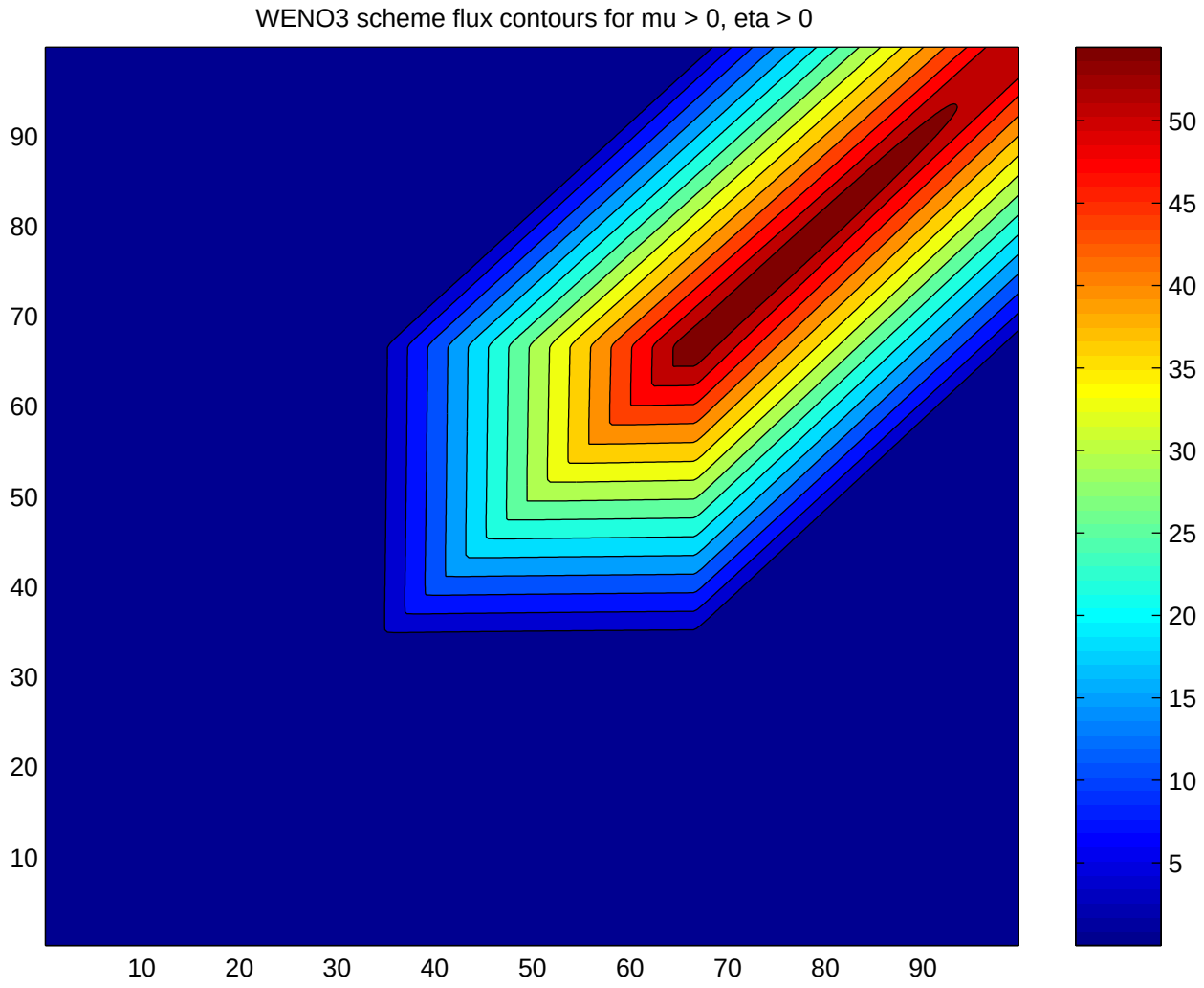
$$\psi(x, 0, t) = 0 \quad \text{for} \quad \Omega_y > 0$$

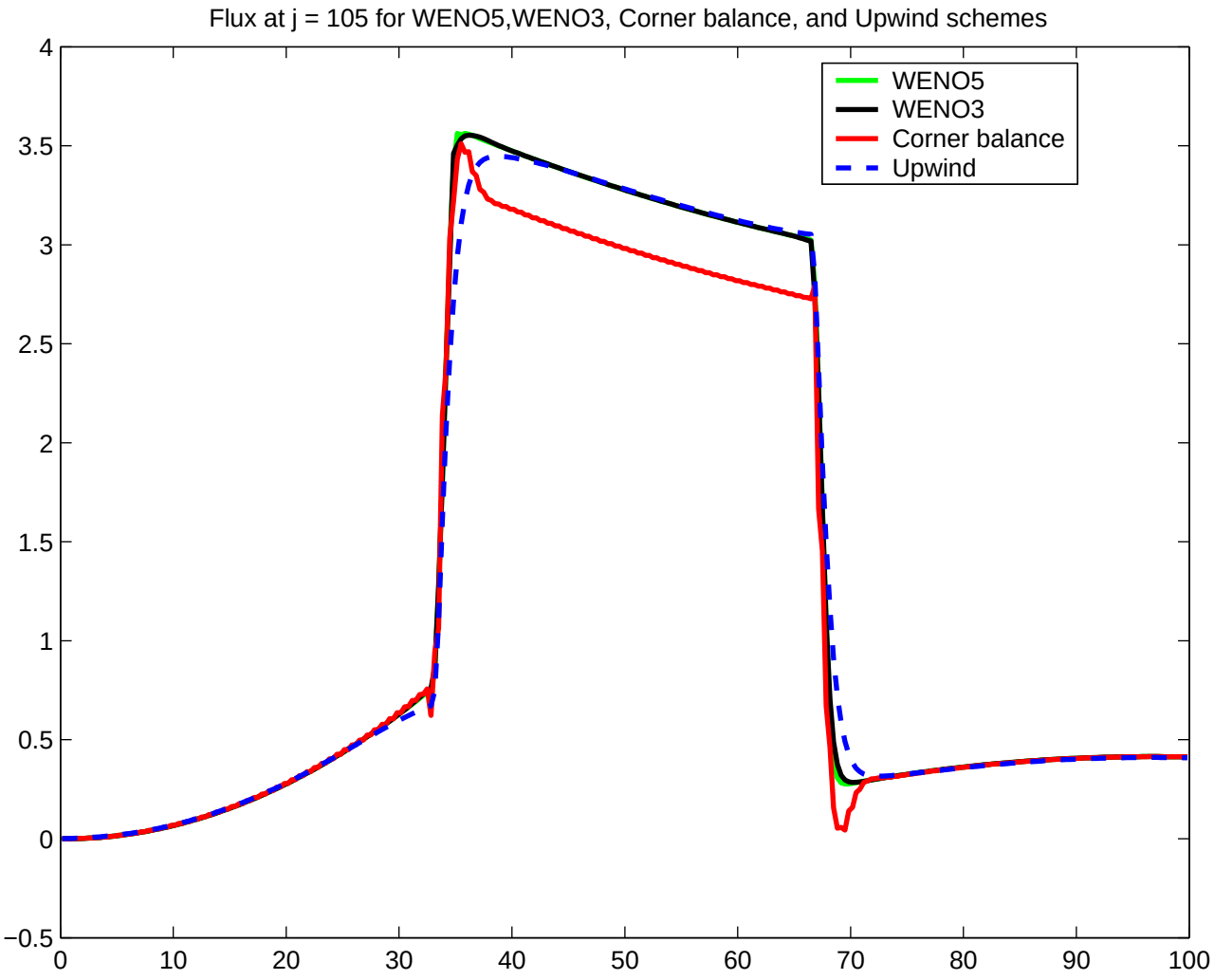
$$\psi(x, 100, t) = 0 \quad \text{for} \quad \Omega_y < 0$$

- $\sigma = 0.001$, $\sigma_s = 0.001$
-

$$q = \begin{cases} 1, & \text{if } (x, y) \in [33.25, 66.75] \times [33.25, 66.75] \\ 0, & \text{otherwise} \end{cases}$$

- $N_x = 300$, $N_y = 300$
- Steady-state simulation: used KINSOL as nonlinear solver.
- Compared WENO3 to:
  (i) Corner-balance method (cell centered)
  (ii) 1st order upwind scheme (node centered)


WENO3 scheme flux contours for mu > 0, eta > 0
90
80
70
60
50
40
30
20
10
10
20
30
40
50
60
70
80
90
50
45
40
35
30
25
20
15
10
5

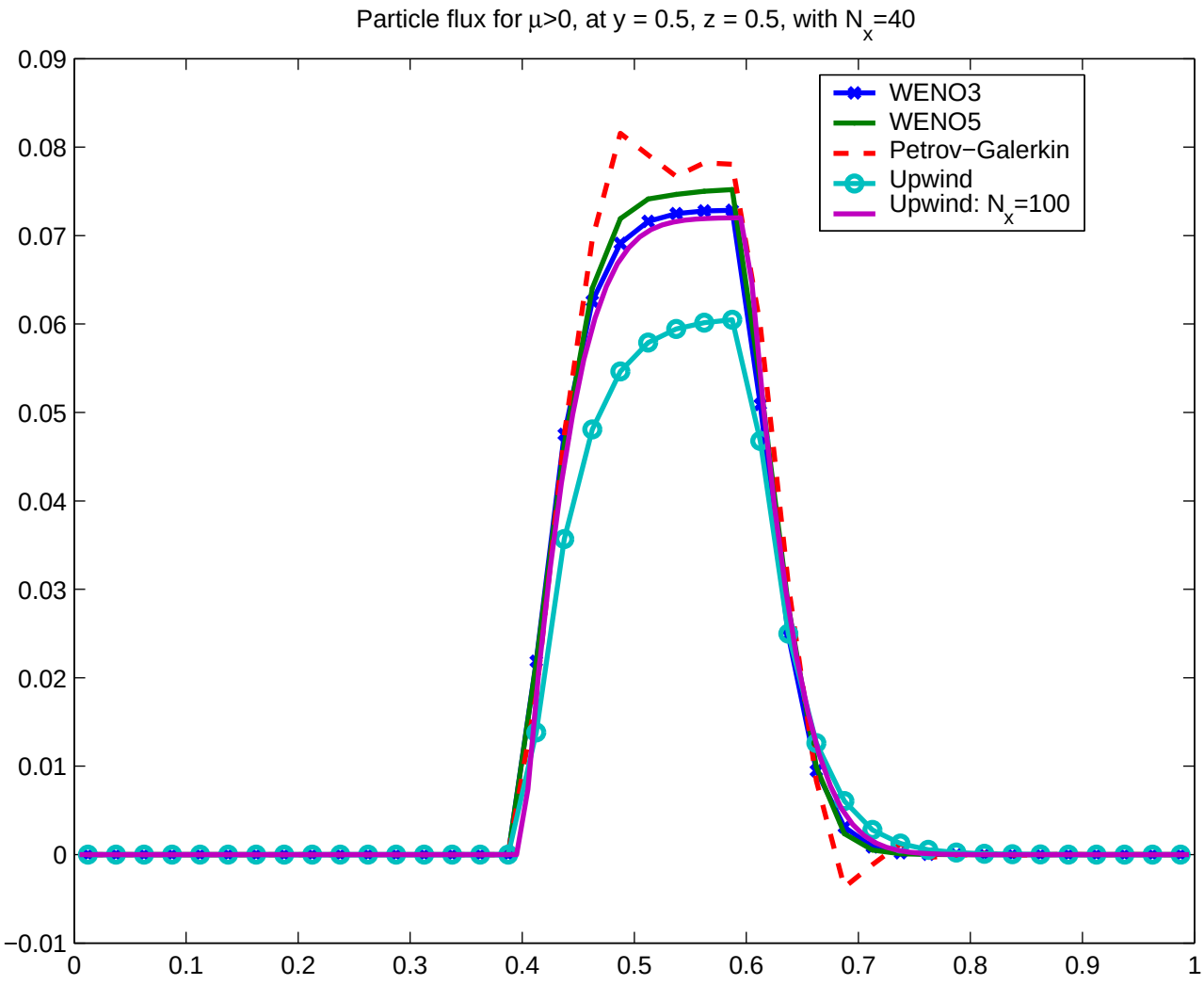

Flux at j = 105 for WENO5,WENO3, Corner balance, and Upwind schemes
WENO5
WENO3
Corner balance
Upwind
4
3.5
3
2.5
2
1.5
1
0.5
0
−0.5
0
10
20
30
40
50
60
70
80
90
100

3-D TEST PROBLEM

- IC: $\psi_0(x, y, z) = 0$ for $(x, y, z) \in [0, 1] \times [0, 1] \times [0, 1]$ at $t = 0$.
- Dirichlet BC at "inflow":

$$\begin{aligned}
\psi(0, y, z, t) &= 0 \quad \text{for} \quad \Omega_x > 0 \\
\psi(1, y, z, t) &= 0 \quad \text{for} \quad \Omega_x < 0 \\
\psi(x, 0, z, t) &= 0 \quad \text{for} \quad \Omega_y > 0 \\
\psi(x, 1, z, t) &= 0 \quad \text{for} \quad \Omega_y < 0 \\
\psi(x, y, 0, t) &= 0 \quad \text{for} \quad \Omega_z > 0 \\
\psi(x, y, 1, t) &= 0 \quad \text{for} \quad \Omega_z < 0
\end{aligned}$$

- $\sigma = 10.$, $\sigma_s = 0$
- $$q = \begin{cases} 1, & \text{if } (x, y, z) \in [.4, .6] \times [.4, .6] \times [.4, .6] \\ 0, & \text{otherwise} \end{cases}$$
- $N_x = 40$, $N_y = 40$, $N_z = 40$
- Steady-state simulation: used KINSOL as nonlinear solver.
- Compared WENO3 and WENO5 to:
  (i) Petrov-Galerkin (node centered)
  (ii) 1st order upwind scheme (node centered)
  (iii) 1st order upwind on fine grid ($100 \times 100 \times 100$)


Particle flux for μ>0, at y = 0.5, z = 0.5, with N_x=40
WENO3
WENO5
Petrov−Galerkin
Upwind
Upwind: N_x=100
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
−0.01
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

CONCLUDING REMARKS

- ENO/WENO schemes offer a non-oscillatory spatial discretization.
- Reduces/eliminates oscillations near true discontinuities, as well as steep gradients.
- Could be used for both *linear* and *nonlinear* governing equations.
- Could be used with both *finite difference* and it finite volume methods.
- Comparable cost for scalar problems.
- Recommended for unsteady problems with large parts of smooth variation/features and discontinuous material interfaces.
- Has advantages for steady-state problems as well.