A Particle Method for Conservation Law PDEs

Yossi Farjoun[1] Benjamin Seibold[2]

[1]G. Millán Institute of Fluid Dynamics, Nanoscience and Industrial Mathematics, UC3M

[2]Department of Mathematics, Temple University

July 7th, 2010
Duke University

Universidad Carlos III de Madrid

The Problem

- Conservation laws
- Grid methods
- Particle methods
- Properties of solutions

Our Method

- Advantages and limitations of particles
- Find interpolation between particles
- Define basic method
- Extensions
- Examples
- Future work

Conservation Law PDE

$$u_t + f(u)_x = 0, \qquad u(x,0) = u_0(x) \tag{1}$$

With many possible modifications:

1. Multiple space dimensions
2. System of equations
3. Non-zero RHS (“Balance Equations”)
4. Explicit dependence on x
5. Non-constant “Capacity”, multiplier of $t-$derivative term
6. Inclusion of derivatives of u, for example, the heat equation

Examples of conservative PDE

1. Non-linear advection (Burgers' equation) $u_t + (\frac{1}{2}u^2)_x = 0$
2. Traffic flow $u_t + (V(u)u)_x = 0$
3. Two-phase flow (Buckley-Leverett Equation) $u_t + (\frac{u^2}{u^2+a(1-u)})_x = 0$
4. Reactive flow $u_t + (\frac{1}{2}u^2)_x = g(u)$
5. Shallow water equations $$\begin{pmatrix} h \\ uh \end{pmatrix}_t + \begin{pmatrix} uh \\ hu^2 + \frac{1}{2}gh^2 \end{pmatrix}_x = 0$$
6. Euler equations $$\begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (E+p)u \end{pmatrix}_x = 0$$

The *cons* of fixed grid methods

- Simulate sideways motion by an up-down motion
- Require a continuous estimate of the local derivatives
- Cell-average as the basic datum, implies smearing of data
- *A priori* determination of grid, without knowing the solution
- Step-size is determined by the largest velocity

The *pros* of fixed grid methods

- Somewhat easier to code
- Implementation for higher-dimension and systems relatively clear
- Conservation properties transfer easily

The *cons* of particle methods

- Unclear how to deal with overtaking particles and “gaps” in a conservative way
- Implementation for higher-dimension and systems unknown

The *pros* of particle methods

- Naturally follow function values rather than averages
- Easily adjust local resolution according to solution
- Step-size not dependent on the velocity itself but rather on its change

The *cons* of particle methods

- Unclear how to deal with overtaking particles and “gaps” in a conservative way (until now...)
- Implementation for higher-dimension and systems unknown

The *pros* of particle methods

- Naturally follow function values rather than averages
- Easily adjust local resolution according to solution
- Step-size not dependent on the velocity itself but rather on its change

The *cons* of particle methods

- Unclear how to deal with overtaking particles and “gaps” in a conservative way (until now...)
- Implementation for higher-dimension and systems unknown (still...)

The *pros* of particle methods

- Naturally follow function values rather than averages
- Easily adjust local resolution according to solution
- Step-size not dependent on the velocity itself but rather on its change

Properties of conservation law

Let us start with the simple conservation law $u_t + f(u)_x = 0$

By integrating we understand why f is called the flux function

$$\frac{\partial}{\partial t}\int_a^b u(x,t)\,dx = \int_a^b u_t\,dx = -\int_a^b f(u)_x = f(u(a)) - f(u(b))$$

Properties of conservation law

Let us start with the simple conservation law $u_t + f(u)_x = 0$

By integrating we understand why f is called the flux function

$$\frac{\partial}{\partial t}\int_a^b u(x,t)\,dx = \int_a^b u_t\,dx = -\int_a^b f(u)_x = f(u(a)) - f(u(b))$$

Characteristics, however, are found by differentiation

$$\frac{du(x(t),t)}{dt} = \dot{x}u_x + u_t = (\dot{x} - f'(u))u_x$$

So if $\dot{x} = f'(u)$ we have constant u on characteristics

Using characteristic particles

The area between characteristic particles

Assuming that $x_1(t)$ and $x_2(t)$ are the locations of characteristic particles (that is they satisfy $\dot{x}_i(t) = f'(u(x_i, t)) = f'(u_i)$) we can look at the change of area between them:

$$\frac{d}{dt}\int_{x_1(t)}^{x_2(t)} u\,dx = \int_{x_1}^{x_2} u_t\,dx + \dot{x}_2 u_2 - \dot{x}_1 u_1$$

Using characteristic particles

The area between characteristic particles

Assuming that $x_1(t)$ and $x_2(t)$ are the locations of characteristic particles (that is they satisfy $\dot{x}_i(t) = f'(u(x_i, t)) = f'(u_i)$) we can look at the change of area between them:

$$\frac{d}{dt}\int_{x_1(t)}^{x_2(t)} u\,dx = \int_{x_1}^{x_2} u_t\,dx + \dot{x}_2 u_2 - \dot{x}_1 u_1$$
$$= f(u)|_{u_1}^{u_2} - f'(u)u|_{u_1}^{u_2} = F(u)|_{u_1}^{u_2}$$

where F is the Legendre transform of f: $F(u) = f'(u)u - f(u)$

Using characteristic particles

The area between characteristic particles

Assuming that $x_1(t)$ and $x_2(t)$ are the locations of characteristic particles (that is they satisfy $\dot{x}_i(t) = f'(u(x_i, t)) = f'(u_i)$) we can look at the change of area between them:

$$\frac{d}{dt}\int_{x_1(t)}^{x_2(t)} u\,dx = \int_{x_1}^{x_2} u_t\,dx + \dot{x}_2 u_2 - \dot{x}_1 u_1$$
$$= f(u)|_{u_1}^{u_2} - f'(u)u|_{u_1}^{u_2} = F(u)|_{u_1}^{u_2}$$

where F is the Legendre transform of f: $F(u) = f'(u)u - f(u)$

While different than for the constant $x-$location, it is also a constant

Distance between x_1 and x_2

$$\dot{x}_i = f(u_i) \Rightarrow \frac{d}{dt}(x_2 - x_1) = f'(u)\big|_{u_1}^{u_2}$$

which is constant as well!

Distance between x_1 and x_2

$$\dot{x}_i = f(u_i) \Rightarrow \frac{d}{dt}(x_2 - x_1) = f'(u)|_{u_1}^{u_2}$$

which is constant as well!

Thus $\exists t_0$ (greater or smaller than t) s.t.

$$\int_{x_1(t)}^{x_2(t)} u(x,t)\,dx = (t - t_0) \cdot F(u)|_{u_1}^{u_2},$$
$$x_2(t) - x_1(t) = (t - t_0) \cdot f'(u)|_{u_1}^{u_2}.$$

Distance between x_1 and x_2

$$\dot{x}_i = f(u_i) \Rightarrow \frac{d}{dt}(x_2 - x_1) = f'(u)|_{u_1}^{u_2}$$

which is constant as well!

Thus $\exists t_0$ (greater or smaller than t) s.t.

$$\int_{x_1(t)}^{x_2(t)} u(x,t)\,dx = (t - t_0) \cdot F(u)|_{u_1}^{u_2},$$
$$x_2(t) - x_1(t) = (t - t_0) \cdot f'(u)|_{u_1}^{u_2}.$$

And thus

$$\int_{x_1(t)}^{x_2(t)} u(x,t)\,dx = (x_2 - x_1) \cdot a(u_1, u_2)$$

with

$$a(v,w) = \frac{F(u)|_v^w}{f'(u)|_v^w} = \frac{\int_v^w f''(u) \cdot u\,du}{\int_v^w f''(u)\,du}$$

Properties of $a(v,w) = \frac{\int_v^w f''(u) \cdot u \, du}{\int_v^w f''(u) \, du}$

For a convex (or concave) f we have the following

Lemma

The function $a(v,w)$ is

1. *the same for f and $-f$*
2. *symmetric in v and w*
3. *an average (i.e. $a(v,w) \in (v,w)$)*
4. *strictly increasing*
5. *continuous with $a(v,v) = v$*

Properties of $a(v,w) = \frac{\int_v^w f''(u)\cdot u\,du}{\int_v^w f''(u)\,du}$

For a convex (or concave) f we have the following

Lemma

The function $a(v,w)$ is

1. *the same for f and $-f$*
2. *symmetric in v and w*
3. *an average (i.e. $a(v,w) \in (v,w)$)*
4. *strictly increasing*
5. *continuous with $a(v,v) = v$*

Recall that

$$a(v,w) = \frac{\int_v^w f''(u)\cdot u\,du}{\int_v^w f''(u)\,du}$$

Proof of item 4.

Assume WLOG that $v < w < z$ and that $f'' > 0$

$$a(v,z) = \frac{\int_v^w f''(u)u\,du + \int_w^z f''(u)u\,du}{\int_v^z f''(u)\,du} \tag{2}$$

$$> \frac{a(v,w)\int_v^w f''(u)\,du + a(v,w)\int_w^z f''(u)\,du}{\int_v^z f''(u)\,du} = a(v,w) \tag{3}$$

which proves that $a(\cdot,\cdot)$ is increasing in the second argument. □

Recall that

$$a(v,w) = \frac{\int_v^w f''(u)\cdot u\,du}{\int_v^w f''(u)\,du}$$

Proof of item 4.

Assume WLOG that $v < w < z$ and that $f'' > 0$

$$a(v,z) = \frac{\int_v^w f''(u)u\,du + \int_w^z f''(u)u\,du}{\int_v^z f''(u)\,du} \tag{2}$$

$$> \frac{a(v,w)\int_v^w f''(u)\,du + a(v,w)\int_w^z f''(u)\,du}{\int_v^z f''(u)\,du} = a(v,w) \tag{3}$$

which proves that $a(\cdot,\cdot)$ is increasing in the second argument. □

Recall that

$$a(v,w) = \frac{\int_v^w f''(u)\cdot u\,du}{\int_v^w f''(u)\,du}$$

Proof of item 4.

Assume WLOG that $v < w < z$ and that $f'' > 0$

$$a(v,z) = \frac{\int_v^w f''(u)u\,du + \int_w^z f''(u)u\,du}{\int_v^z f''(u)\,du} \tag{2}$$

$$> \frac{a(v,w)\int_v^w f''(u)\,du + a(v,w)\int_w^z f''(u)\,du}{\int_v^z f''(u)\,du} = a(v,w) \tag{3}$$

which proves that $a(\cdot,\cdot)$ is increasing in the second argument. □

Rankine-Hugoniot condition: A reminder

If a shock exists between two (fixed) points $a < x_s(t) < b$ we can integrate the equation to find

The shock speed

$$\frac{d}{dt}\left(\int_a^{x_s(t)} u\,dx + \int_{x_s(t)}^b u\,dx\right) = -\int_a^b f(u)_x\,dx$$

Therefore

$$\dot{x}\cdot\left\{u^-(x_s(t)) - u^+(x_s(t))\right\} = f(u^-) - f(u^+)$$

which gives

$$s = \dot{x} = \frac{[f]}{[u]}$$

The Particle Method

The particle method (short version)

- Keep list of particles and function values $\{(x_i, u_i)\}$
- Choose time-step, Δt
- Move particles according to characteristics $\tilde{x}_i = x_i + \Delta t\, f'(u_i)$
- Merge neighboring particles that are close enough
- Add new particles into large gaps

Due to the characteristics, the particles are quite easy to follow however, several questions remain:

Questions about particles

- Exactly what to do when particles “collide”?
- Exactly what to do when a gap forms?
- How to initialize the particles from the initial conditions?
- What is the function value between the particles?
- What if the flux function has an inflection point?
- How to deal with a source term?
- Do we get entropy solutions?

Due to the characteristics, the particles are quite easy to follow however, several questions remain:

Questions about particles

- Exactly what to do when particles "collide"?
- Exactly what to do when a gap forms?
- How to initialize the particles from the initial conditions?
- What is the function value between the particles?
- What if the flux function has an inflection point?
- How to deal with a source term?
- Do we get entropy solutions?

Our answer to most of these questions comes from discovering a natural interpolation between the particles.

What happens when $t = t_0$?

Recall that we said that $\exists t_0$ (greater or smaller than t) s.t.

$$\int_{x_1(t)}^{x_2(t)} u(x,t)\,dx = (t - t_0) \cdot F(u)|_{u_1}^{u_2},$$
$$x_2(t) - x_1(t) = (t - t_0) \cdot f'(u)|_{u_1}^{u_2}.$$

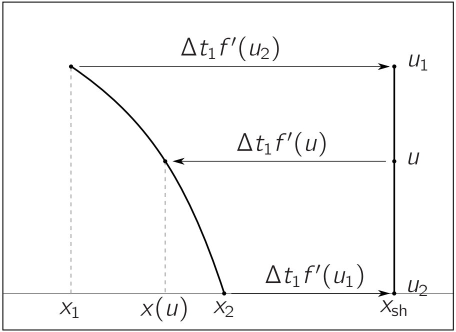
Thus, at $t = t_0$ we must have a shock. To find the interpolation, we solve from t_0 to t:

What happens when $t = t_0$?

Recall that we said that $\exists t_0$ (greater or smaller than t) s.t.

$$\int_{x_1(t)}^{x_2(t)} u(x,t)\,dx = (t - t_0) \cdot F(u)|_{u_1}^{u_2},$$
$$x_2(t) - x_1(t) = (t - t_0) \cdot f'(u)|_{u_1}^{u_2}.$$

Thus, at $t = t_0$ we must have a shock. To find the interpolation, we solve from t_0 to t:



The inter-particle interpolation

$$x(u) = x_1 + \frac{f'(u) - f'(u_1)}{f'(u_2) - f'(u_1)}(x_2 - x_1)$$

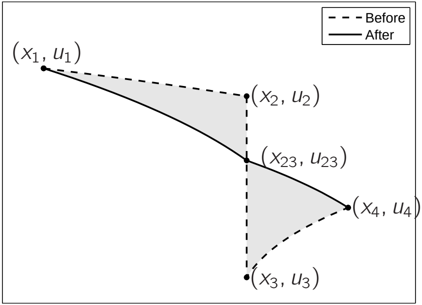
The inter-particle interpolation

$$x(u) = x_1 + \frac{f'(u) - f'(u_1)}{f'(u_2) - f'(u_1)}(x_2 - x_1)$$

Which allows us to easily insert and merge particles as needed.

Insert by placing a particle on the interpolation

Merge by replacing the two particles with one so that area gained is equal to the area lost



Some more properties

Merging particles

- Has a unique solution
- New particle is bounded by its neighbors

Some more properties

Merging particles

- Has a unique solution
- New particle is bounded by its neighbors

The interpolation function

- Is an analytic solution of the PDE
- Provides a consistent function to use with a source term

Some more properties

Merging particles

- Has a unique solution
- New particle is bounded by its neighbors

The interpolation function

- Is an analytic solution of the PDE
- Provides a consistent function to use with a source term

Resulting method is

- Total Variation Diminishing (TVD)
- Entropy non-increasing
- Provides means for determining the existence and location of shocks

Some more properties

Merging particles

- Has a unique solution
- New particle is bounded by its neighbors

The interpolation function

- Is an analytic solution of the PDE
- Provides a consistent function to use with a source term

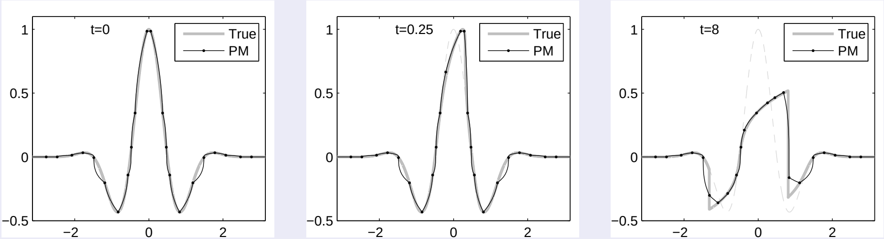
Resulting method is

- Total Variation Diminishing (TVD)
- Entropy non-increasing
- Provides means for determining the existence and location of shocks
- Has 2^{nd} order accuracy, even near shocks

A first example

Flux function: $f(u) = \frac{1}{4}u^4$

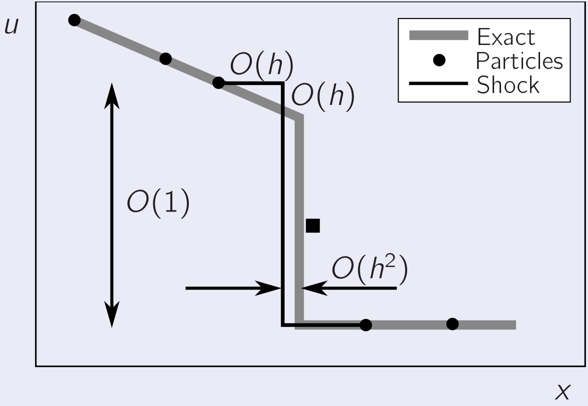
Using initial conditions $u(x,0) = e^{-x^2}\cos\pi x$ and about 20 particles



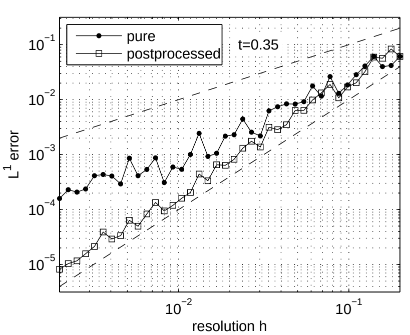
Post-processing: shock detection

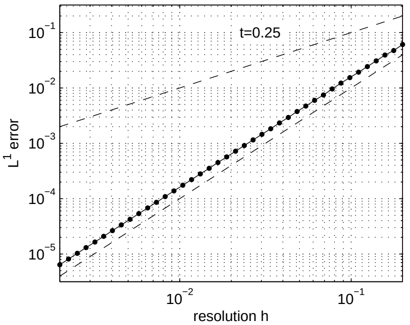
The idea is simple: the location of a shock is determined by its height and the area "under" it

A sketch of shock detection



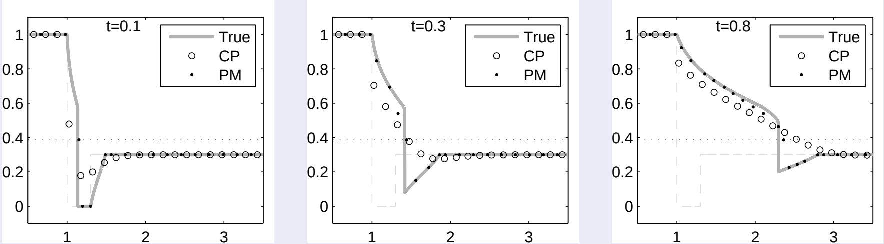
Accuracy tests





We extend the method to allow for inflection points.

Buckley-Leverett Equation



Flux function is $f(u) = \dfrac{u^2}{u^2 + \frac{1}{2}(1-u)^2}$

Another example: Burger's with a soft source-term

We consider a flow over an obstacle

$$u_t + uu_x = b'(x)u, \qquad b(x) = \begin{cases} \cos(\pi x) & x \in [4.5, 5.5] \\ 0 & \text{otherwise} \end{cases}$$

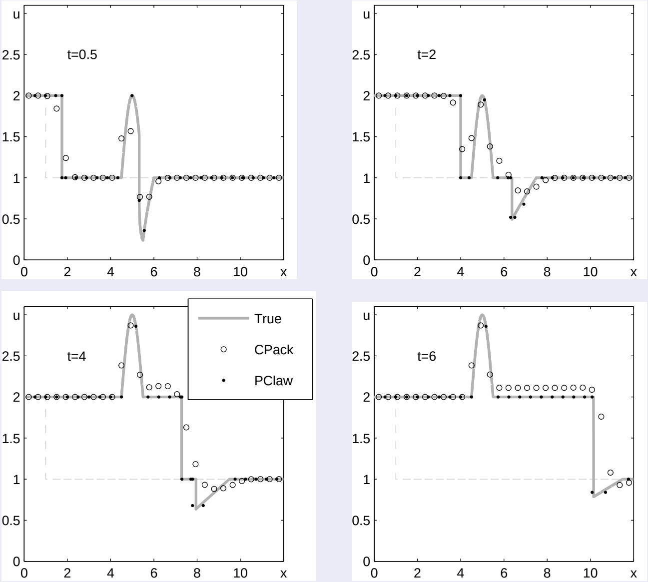
Since there is a non-zero source term, the function value u_i is not constant. The characteristic equations are therefore

Characteristic equations

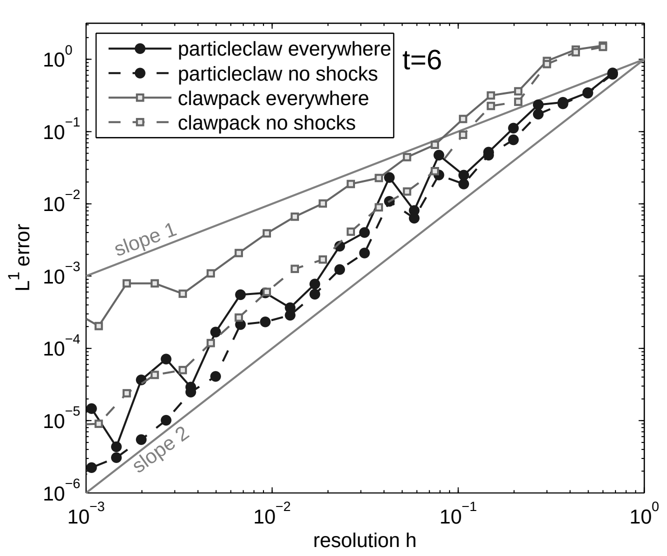
$$\dot{x}_i = f'(u) = u_i$$
$$\dot{u}_i = g(x, u) = u_i b'(x_i)$$

Which can be solved using an ODE solver. Problem is that where the source is active, the similarity solutions are no longer analytical solutions and therefore the conservation argument is only approximate.

Flow over an obstacle



L^1 Error, with CLAWPACK of Flow over an obstacle



Another extension—An "Exact" solver

Motivation

The PDE

$$u_t + uu_x = \frac{1}{\tau} u(1-u)(u-\beta), \qquad \tau \ll 1, \qquad 0 < \beta < 1$$

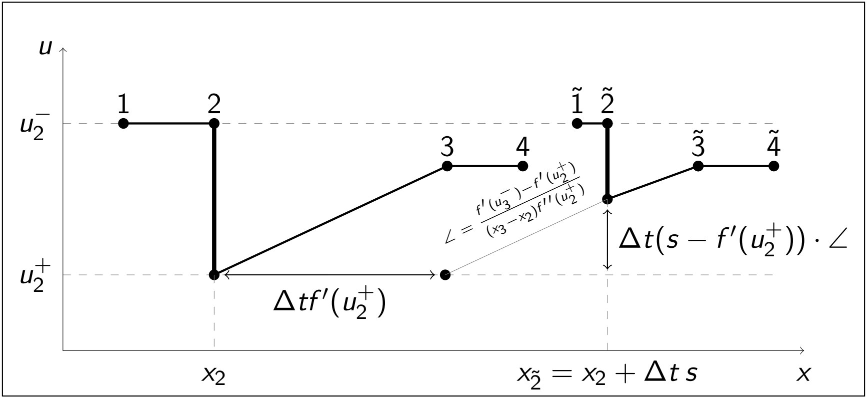
as a model for reaction + nonlinear advection.

Why difficult?

- Stiff source term
- Sharp transitions in solution
- Need to resolve fronts to get correct source term

The extension changes the definition of the particles

Now, particles have 2 function values: x_i, u_i^+, u_i^- and follow the motion of shocks



Exact method

Equations of motion

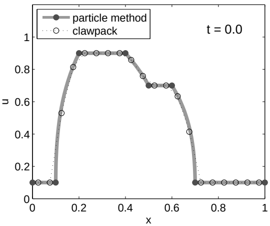
$$\dot{x}_i = s = \begin{cases} \frac{f(u_i^+)-f(u_i^-)}{u_i^+-u_i^-} & u_i^+ \neq u_i^- \\ f'(u_i) & u_i^+ = u_i^- \end{cases}$$

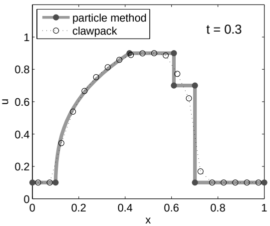
$$\dot{u}_i^\pm = (\dot{x}_i - f'(u_i^\pm))\frac{f'(u_{i\pm 1}^\mp) - f'(u_i^\pm)}{x_{i\mp 1} - x_i}\frac{1}{f''(u_i^\pm)}$$

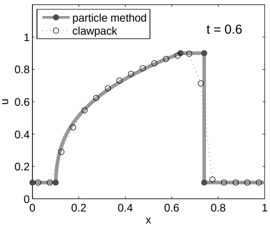
Solve using your favorite ODE solver and get the accuracy of the solver..

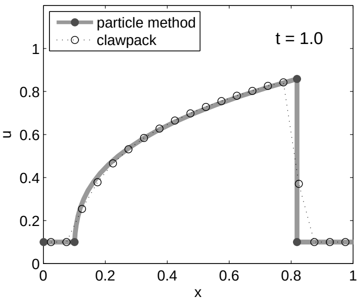
What does “exact” mean, exactly?

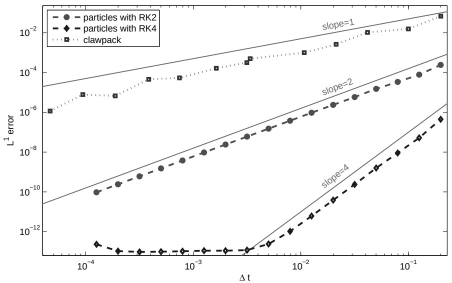
Solve $u_t + f(u)_x = 0$ with $f(u) = \frac{1}{4}u^4$











And finally...the stiff problem

$$u_t + uu_x = \frac{1}{\tau} u(1-u)(u-\beta), \qquad \tau \ll 1, \qquad 0 < \beta < 1$$

Problem

Particles quickly move towards 1 or 0 and no source is generated

And finally...the stiff problem

$$u_t + uu_x = \frac{1}{\tau} u(1-u)(u-\beta), \qquad \tau \ll 1, \qquad 0 < \beta < 1$$

Problem

Particles quickly move towards 1 or 0 and no source is generated

Solution

Add a special particle at β and treat neighboring particles specially: Calculate required change to area and move neighboring particles horizontally to create this additional area.

And finally...the stiff problem

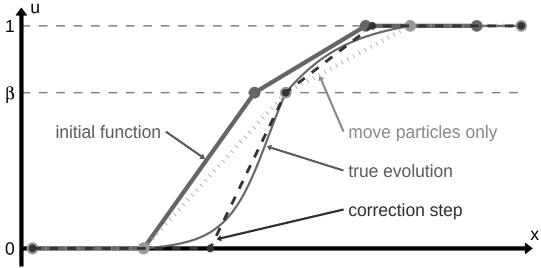
$$u_t + uu_x = \frac{1}{\tau} u(1-u)(u-\beta), \qquad \tau \ll 1, \qquad 0 < \beta < 1$$

Problem

Particles quickly move towards 1 or 0 and no source is generated

Solution

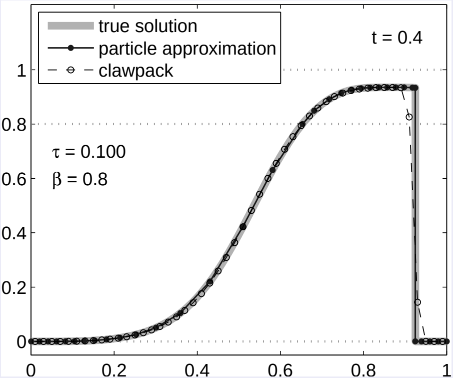
Add a special particle at β and treat neighboring particles specially: Calculate required change to area and move neighboring particles horizontally to create this additional area.



Numerical Simulation

$$u_t + uu_x = \frac{1}{\tau}u(1-u)(u-\beta), \qquad \tau \ll 1, \qquad 0 < \beta < 1$$

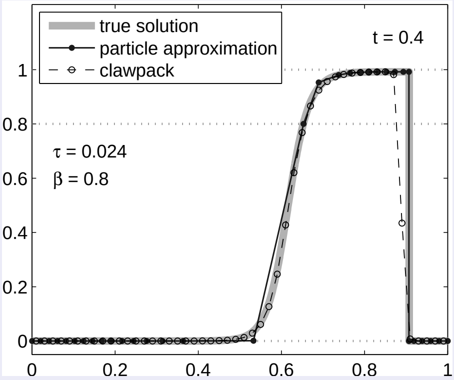
In comparison to CLAWPACK



Numerical Simulation

$$u_t + uu_x = \frac{1}{\tau}u(1-u)(u-\beta), \qquad \tau \ll 1, \qquad 0 < \beta < 1$$

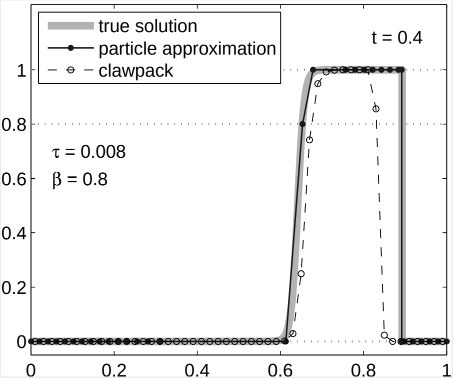
In comparison to CLAWPACK



Numerical Simulation

$$u_t + uu_x = \frac{1}{\tau}u(1-u)(u-\beta), \qquad \tau \ll 1, \qquad 0 < \beta < 1$$

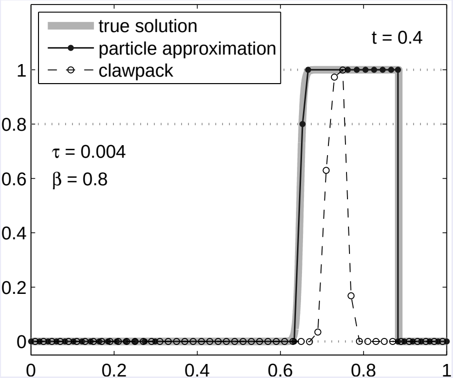
In comparison to CLAWPACK



Numerical Simulation

$$u_t + uu_x = \frac{1}{\tau}u(1-u)(u-\beta), \qquad \tau \ll 1, \qquad 0 < \beta < 1$$

In comparison to CLAWPACK



Conclusions and Future directions

"Take-home" Message

Conclusions and Future directions

"Take-home" Message

- A "natural" solution can answer many questions

Conclusions and Future directions

“Take-home” Message

- A “natural” solution can answer many questions
- Particle methods are flexible and allow problem-specific “hacks”

Conclusions and Future directions

“Take-home” Message

- A “natural” solution can answer many questions
- Particle methods are flexible and allow problem-specific “hacks”

Current projects

Conclusions and Future directions

"Take-home" Message

- A "natural" solution can answer many questions
- Particle methods are flexible and allow problem-specific "hacks"

Current projects

- Traffic flow on a large network

Conclusions and Future directions

“Take-home” Message

- A “natural” solution can answer many questions
- Particle methods are flexible and allow problem-specific “hacks”

Current projects

- Traffic flow on a large network
- Non-linear flow with a convolution source term.

Conclusions and Future directions

"Take-home" Message

- A "natural" solution can answer many questions
- Particle methods are flexible and allow problem-specific "hacks"

Current projects

- Traffic flow on a large network
- Non-linear flow with a convolution source term.

Future extensions

Conclusions and Future directions

"Take-home" Message

- A "natural" solution can answer many questions
- Particle methods are flexible and allow problem-specific "hacks"

Current projects

- Traffic flow on a large network
- Non-linear flow with a convolution source term.

Future extensions

- Move particles perpendicular to solution?

Conclusions and Future directions

"Take-home" Message

- A "natural" solution can answer many questions
- Particle methods are flexible and allow problem-specific "hacks"

Current projects

- Traffic flow on a large network
- Non-linear flow with a convolution source term.

Future extensions

- Move particles perpendicular to solution?
- Follow area between particles to refine better?

Conclusions and Future directions

"Take-home" Message

- A "natural" solution can answer many questions
- Particle methods are flexible and allow problem-specific "hacks"

Current projects

- Traffic flow on a large network
- Non-linear flow with a convolution source term.

Future extensions

- Move particles perpendicular to solution?
- Follow area between particles to refine better?

Pipe Dreams

Conclusions and Future directions

"Take-home" Message

- A "natural" solution can answer many questions
- Particle methods are flexible and allow problem-specific "hacks"

Current projects

- Traffic flow on a large network
- Non-linear flow with a convolution source term.

Future extensions

- Move particles perpendicular to solution?
- Follow area between particles to refine better?

Pipe Dreams

- Develop method for systems

Conclusions and Future directions

"Take-home" Message

- A "natural" solution can answer many questions
- Particle methods are flexible and allow problem-specific "hacks"

Current projects

- Traffic flow on a large network
- Non-linear flow with a convolution source term.

Future extensions

- Move particles perpendicular to solution?
- Follow area between particles to refine better?

Pipe Dreams

- Develop method for systems
- Develop method for higher space dimension

Thank-You!