GAMM 2003 Padua

Van der Waals Models Extended Formulations and Fully Discrete Entropy Satisfying Schemes

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- Motivation

Large Direct Numerical Simulation
of liquid-vapor flows with phase changes
$\hookrightarrow$ Thermodynamic theory of
artificially enlarged interfaces

Sharp control of
the discrete entropy balance equation

- Considerable attention over the past years

  Abeyaratne and Knowles

$\star$ Truskinovsky

$\star$ Gavriliuk, Gavrilyuk and Gouin

Jamet, Jamet-Lebaigue

Shearer et al.

$\star$ LeFloch

Slemrod

Serre

Benzoni

Xin

$\star$ Cockburn-Gau

$\star$ LeFloch-Rohde

$\star$ Chalons-LeFloch

and many other contributions…

- Outlook

$\longrightarrow$ The PDE model :

Energy(density, Entropy, ∇ density) and the
Entropy condition :
The Interstitial Work

$\hookrightarrow$ *Strong Departure* from the Gas Dynamics setting

$\longrightarrow$ An Extended PDE system that encodes the original model

Prescribing appropriate initial data
yields solutions of the original PDE's

$\hookrightarrow$ The original entropy condition is preserved

$\longrightarrow$ The numerical method

Splitting technique :
from Gas Dynamics to Interstitial Work

$\hookrightarrow$ Fully discrete cell-entropy inequalities
under a natural CFL condition

A Rough Guideline

PDEs with Viscous-Cappilar regularization :

$$\partial_t \mathbf{u}^\epsilon + \nabla.\mathcal{F}(\mathbf{u}^\epsilon) = \nabla.\mathcal{R}(\epsilon \nabla \mathbf{u}^\epsilon,\ \epsilon^2 \nabla^2 \mathbf{u}^\epsilon), \quad t > 0,\ x \in I\!R^d$$

Regularization sensitive solutions

Phase transition :

$(\mathbf{v}_{-\infty}, \mathbf{v}_{+\infty}; \sigma)_{\frac{\sqrt{(\lambda)}}{\mu}}$

The Entropy encodes sensitivity :

$$\rho D_t s = \partial_t \rho s + \nabla.\rho s \mathbf{u} = \Phi(\frac{\sqrt{(\lambda)}}{\mu}) < 0$$

$\hookrightarrow$ Control $\rho D_t s$!

Difficulty : $s = s(\mathbf{u}, \epsilon \nabla \mathbf{u})$!

$D_t \mathbf{u}$ being discretized then

Control$D_t \nabla \mathbf{u}$ $\hookrightarrow$ Control $D_t s(\mathbf{u}, \epsilon \nabla \mathbf{u})$

Hint : Extended Unknown $\mathbf{w} = (\mathbf{u}, \epsilon \nabla \mathbf{u})$

$$\partial_t \mathbf{w}^\epsilon + \nabla.\mathcal{G}(\mathbf{w}^\epsilon) = \nabla.\mathcal{R}(\epsilon \nabla \mathbf{w}^\epsilon)$$

(1) so that

$$\rho D_t s(\mathbf{w}) = \Phi(\frac{\sqrt{(\lambda)}}{\mu})$$

The PDE model

Let be given $\epsilon > 0$ (scaling parameter)

$$
\begin{aligned}
&\partial_t \rho + \nabla.\rho\mathbf{u} = 0, \quad t > 0,\ x \in I\!R^d \\
&\partial_t \rho\mathbf{u} + \nabla.(\rho\mathbf{u}\otimes\mathbf{u} + p(v,s)I - \epsilon^2\mathcal{T}_{\mathcal{K}}) = \epsilon\nabla.\sigma, \\
&\partial_t E + \nabla.((E + p(v,s))\mathbf{u} - \epsilon^2\mathcal{T}_{\mathcal{K}}\mathbf{u}) = \epsilon\nabla.(\sigma\mathbf{u} + \kappa\nabla T) \\
&\qquad\qquad -\epsilon^2\nabla.(\rho^2\nabla.\mathbf{u}\ \partial_{\nabla\rho} e(\rho, s, \nabla\rho)),
\end{aligned}
$$

(2)

Here the closure relation reads :

$$E = \frac{\rho|\mathbf{u}|^2}{2} + \rho e(\rho, s, \nabla\rho)$$

Strong departure from
the usual Gas Dynamic setting

$\hookrightarrow \rho^2\nabla.\mathbf{u}\ \partial_{\nabla\rho} e(\rho, s, \nabla\rho) =$ Interstitial work

needed to enforce for validity the
second principle of the thermodynamics

$$\partial_t \rho s + \nabla.\rho s\mathbf{u} = -\frac{\epsilon}{T}\Big(\sigma : \nabla\mathbf{u} + \kappa\frac{|\nabla T|^2}{T}\Big) - \epsilon\nabla.(\kappa\frac{\nabla T}{T})$$

with $s = s(\rho, \rho\mathbf{u}, E, \nabla\rho)$

Towards the Augmented Formulation

$$E = \frac{\rho|\mathbf{u}|^2}{2} + \mathcal{E}(\frac{1}{\rho}, s) + \epsilon^2 \frac{\lambda(\rho)}{2}|\nabla\rho|^2, \quad \lambda(\rho) > 0$$

$$\bullet \epsilon^2 \mathcal{T_K} = \epsilon^2 \Big\{\rho\lambda(\rho)\nabla.\nabla\rho + \tfrac{1}{2}\big(\rho\lambda'(\rho) - \lambda(\rho)\big)|\nabla\rho|^2\Big\} I + \lambda(\rho)\big\{|\nabla\rho|^2 I - \nabla\rho \otimes \nabla\rho\big\}$$

$$\bullet \epsilon^2 \mathcal{IW} = \epsilon^2 \rho\lambda(\rho)\nabla.\mathbf{u} \ \times \ \nabla\rho$$

Lemma 1 *Let us define*

$$L : \mathbb{R}_+ \longrightarrow \mathbb{R}_+ \ / \ L'(\rho) = l(\rho) = \sqrt{\frac{\lambda(\rho)}{\rho}},.$$

Introduce the mapping :

$$\Theta : \mathbb{R}_+ \times \mathbb{R}^d \longrightarrow \mathbb{R}^d \ / \ \Theta(\rho, \nabla\rho) := \epsilon\nabla L(\rho),$$

Then

$$E = \rho\frac{|\mathbf{u}|^2}{2} + \mathcal{E}(\frac{1}{\rho}, s) + \rho\frac{|\Theta(\rho, \nabla\rho)|^2}{2},$$

- $\epsilon^2 \mathcal{T_K} = \epsilon\rho^2 l(\rho)\nabla.\Theta \ I + \ \rho\big\{|\Theta|^2 I - \Theta \otimes \Theta\big\}$
- $\epsilon^2 \mathcal{IW} = \epsilon\rho^2 l(\rho)\nabla.\mathbf{u} \ \times \ \Theta(\rho, \nabla\rho)$

Towards the Augmented Formulation

Up to diffusive terms, the original PDEs are :

$$
\begin{aligned}
&\partial_t \rho + \nabla.\rho \mathbf{u} = 0,\\
&\partial_t \rho u_x + \nabla.(\rho u_x \mathbf{u}) + \partial_x(p(v,s) - \rho \Theta_y^2) + \partial_y(\rho \Theta_x \Theta_y) = \\
&\qquad\qquad \epsilon \partial_x(\rho^2 l(\rho) \nabla.\Theta),\\
&\partial_t \rho u_y + \nabla.(\rho u_y \mathbf{u}) + \partial_x(\rho \Theta_x \Theta_y) + \partial_y(p(v,s) - \rho \Theta_x^2) = \\
&\qquad\qquad \epsilon \partial_y(\rho^2 l(\rho) \nabla.\Theta),\\
&\partial_t E + \nabla.((E + p(v,s))\mathbf{u} - \mathcal{T}_{\mathcal{K}} \mathbf{u}) = \\
&\qquad\qquad -\epsilon \nabla.(\rho^2 l(\rho) \nabla.\mathbf{u}\ \Theta),
\end{aligned}
$$

(3)

Lemma 2 *The mapping* $\Theta(\rho, \nabla\rho)$ *obeys :*

$$
\begin{aligned}
\rho \mathbf{D}_t \Theta(\rho, \nabla\rho) + \rho \Theta \nabla \mathbf{u} - \rho \nabla.\mathbf{u}\ \Theta &= \\
&-\epsilon \nabla.(\rho^2 l(\rho) \nabla.\mathbf{u} I),
\end{aligned} \tag{4}
$$

! Consider from now on Θ *as an unknown !*
say θ *equipped with its own PDE*

Augmented PDEs System

Consider

$$
\begin{aligned}
&\partial_t \rho + \nabla.\rho\mathbf{u} = 0,\\
&\rho D_t u_x + \partial_x(p - \rho\theta_y^2) + \partial_y(\rho\theta_x\theta_y) = \epsilon\partial_x(\rho^2 l(\rho)\nabla.\theta),\\
&\rho D_t u_y + \partial_x(\rho\theta_x\theta_y) + \partial_y(p - \rho\theta_x^2) = \epsilon\partial_y(\rho^2 l(\rho)\nabla.\theta),\\
&\rho D_t \theta_x + \rho\theta_y\partial_x u_y - \rho\theta_x\partial_y u_y = -\epsilon\partial_x(\rho^2 l(\rho)\nabla.\mathbf{u}),\\
&\rho D_t \theta_y + \rho\theta_x\partial_y u_x - \rho\theta_y\partial_x u_x = -\epsilon\partial_y(\rho^2 l(\rho)\nabla.\mathbf{u}),\\
&\partial_t E + \nabla.((E+p)\mathbf{u} - \mathcal{T}_{\mathcal{K}}\mathbf{u}) = -\epsilon\nabla.(\rho^2 l(\rho)\nabla.\mathbf{u}\ \theta),
\end{aligned}
$$

(5)

$$\text{with} \quad : E = \frac{\rho|\mathbf{u}|^2}{2} + \rho\mathcal{E}(\tau, s) + \frac{\rho|\theta|^2}{2}$$

Proposition 3 *We have :*

- $$D_t(\frac{1}{\rho}\nabla \times \rho\theta) = 0$$

$\hookrightarrow$ *full conservation form recovered asking :*

$$\nabla \times \rho\theta = 0 \qquad !$$

.

Proposition 4 *Preserved Entropy law :*

- $$-\rho T D_t s(\rho, \mathbf{u}, \theta, E) = \left\{\epsilon\sigma : \nabla\mathbf{u} + \epsilon\nabla.(\kappa\nabla T)\right\}$$

Original Solutions $\in$ Augmented System

Proposition 5 *Let* $\mathbf{w}_0 =^T (\rho,\ \rho\mathbf{u},\ \rho\theta,\ E)$ *:*

$$\theta_0 = \epsilon \nabla L(\rho_0)$$

$\hookrightarrow$ $\mathbf{w}(x,t) =^T (\rho,\ \rho\mathbf{u},\ \rho\theta,\ E)$ *such that :*

$$\theta(x,t) = \epsilon \nabla L(\rho(x,t)), \quad \textit{for all } x,\ t$$

$\hookrightarrow$ $\mathbf{v} :=^T (\rho,\ \rho\mathbf{u},\ E)$ *is nothing but the original solution with data* $\mathbf{v}_0 =^T (\rho_0,\ \rho\mathbf{u}_0,\ E_0)$.

A word About the Eigenstructure

(6)

Numerics : Focusing on Interstitial Work

$\hookrightarrow$ Lagrangian Isothermal setting : $\mathcal{E} = \mathcal{E}(v)$

$\hookrightarrow$ Easy extension to Non Isothermal setting

$$\partial_s \mathcal{E}(v, s) = T > 0$$

Solve for small time strip $t^{n+1} - t^n$ but with appropriate initial data $\theta(y, t^n) = \epsilon L(v(y, t^n))_y$

$$\begin{aligned}
&v_t - u_y = 0, \\
&u_t + (p(v) - \epsilon l(v)\theta_y)_y = \epsilon(\mu u_y)_y, \\
&\theta_t = -\epsilon(l(v)u_y)_y,
\end{aligned}$$

(7)

with additional Energy law

$$\begin{aligned}
E_t + (\mathcal{P}u)_y = {} & \epsilon(\mu u u_y)_y \\
& -\epsilon(\mu u_y^2) - \epsilon(l(v)\theta u_y)_y
\end{aligned}$$

where :

$$E = \frac{1}{2}u^2 + \mathcal{E}(v) + \frac{\theta^2}{2}, \quad \mathcal{P} = p(v) - \epsilon l(v)\theta_y$$

Operator Splitting strategy

• First step : Generalized Gas Dynamic system

$$
\begin{aligned}
&v_t - u_y = 0, \\
(8)\quad &u_t + \mathcal{P}_y = 0, \quad \mathcal{P}(v, \theta_y) = p(v) - \epsilon l(v)(\theta_0)_y \\
&\theta_t = 0,
\end{aligned}
$$

Introduce

$$\hat{\mathcal{E}} = \frac{1}{2}u^2 + \mathcal{E}(v) + \epsilon L(v)(\theta_0)_y, \quad \mathcal{P}(v, (\theta_0)_y) = -\partial_v \hat{\mathcal{E}}_{|u,\theta_y}$$

to get the additional energy law

$$\{\frac{1}{2}u^2 + \mathcal{E}(v) + \epsilon L(v)(\theta_0)_y\}_t + (\mathcal{P}u)_y = 0$$

• Second step : $\hookrightarrow$ Interstitial work

$$v_t = 0, \quad u_t = 0, \quad \theta_t = -\epsilon(l(v)u_y)_y$$

so that combined with the first step

$$\{\frac{u^2}{2} + \mathcal{E}(v) + \frac{\theta^2}{2}\}_t + (\mathcal{P}u)_y = \frac{\theta^2}{2}_t - \epsilon(\theta_0)_y L(v)_t$$

(9)

Restore the Interstitial work ?

Almost Yes : $\quad \dfrac{\theta^2}{2}_t - \epsilon(\theta)_y L(v)_t = -\epsilon(l(v)\theta u_y)_y$

• $\mathbf{v}_{\Delta y}(y,t^n)$ approximate solution

First step : Solve (GD) with I.V. $\mathbf{v}_{\Delta y}(y,t^n)$ so that :

$$(u^2/2+\mathcal{E}(v)+\epsilon\theta_y L(v))(y,t^{n+1})-$$
$$(u^2/2+\mathcal{E}(v)+\epsilon\theta_y L(v))(y,t^{n})+$$
$$\Delta t\times(\mathcal{P}(v,\theta_y)u)_y = \text{Energy Dissipation Rate.}$$

Second Step : Solve :

$$\theta(y,t^{n+1})-\theta(y,t^n)=-\epsilon\Delta t(l(v)u_y)_y,$$

so that as a consequence :

$$(u^2/2+\mathcal{E}(v)+\theta^2/2)(y,t^{n+1})-$$
$$(u^2/2+\mathcal{E}(v)+\theta^2/2)(y,t^{n})+$$
$$\Delta t(\mathcal{P}u)_y+\epsilon\Delta t(\theta l(v)u_y)_y = EDR + Error$$

Enforce $EDR + Error \ \leq 0$ under some suitable CFL condition

• CFL restriction via Fourier Analysis :

$$c^2_{max}=max(-p'(v)+(\frac{\epsilon l(v)}{\Delta y})^2).$$

$\hookrightarrow$ Estimate via sharp cell entropy inequalities

- First step : Energy Dissipation Rate < 0
- Second step : Interstitial work

$$\theta_t = -\epsilon(l(v)u_y)_y$$

For $\Xi \approx l(v)u_y$ to be prescribed, set :

$$\theta_j^{n+1} = \theta_j^n - \epsilon\frac{\Delta t}{\Delta y}(\Xi_{j+1/2}^n - \Xi_{j-1/2}^n)$$

Next to approximate the interstitial work in

$$E_t + (\mathcal{P}u)_y = -\epsilon(\theta \times l(v)u_y)$$

define the limiting function $\beta : I\!R \to [0,1]$:

$$\beta(r) = max(0, \frac{1}{2}\frac{r(r-1)}{r^2+1}), \qquad \text{for all } r \in I\!R$$

and approximate the interstitial work flux $\epsilon(\theta \times l(v)u_y)$ by :

$$\epsilon\Big((1-\beta(r_j^n))\theta_j^n + \beta(r_j^n)\theta_j^{n+1}\Big) \times \Xi_{j+1/2}^n,$$

$$\text{where } r_j^n := \frac{\Xi_{j+1/2}^n}{\Xi_{j-1/2}^n}. \tag{10}$$

Proposition 6

$$\begin{aligned}
&\Delta_t(u^2/2 + \mathcal{E}(v) + \tfrac{\theta^2}{2})_j^{n+1} + \\
&\tfrac{\Delta t}{\Delta y}\Delta_y((\mathcal{P}u)^n_{j+1/2} + \{\epsilon\theta l(v)u_y\}^n_{j+1/2}) \\
(11) = \ & EDR^n_j + \\
&\theta^n_{y\,j}\epsilon\big((L(v_j^{n+1}) - L(v_j^n)) - \Delta t\Xi^n_{j-1/2}\big) + \\
&\big(\epsilon\tfrac{\Delta t}{\Delta y}\big)^2\big(\Xi^n_{j-1/2}\big)^2 \times (b(r^n_j) + b(r^n_{j-1})),
\end{aligned}$$

where $b\ :\ I\!R \longrightarrow [0,1]$ *reads :*

$$b(r) = \frac{1}{2}\frac{(r-1)^2}{r^2+1}, \qquad \textit{for all } r \in I\!R.$$

Remark 7

- $L(v)_t - l(v)u_y = 0$ so that

$$L(v_j^{n+1}) - L(v_j^n) - \Delta t\Xi^n_{j-1/2} \approx 0$$

- $\big(\epsilon\Xi^n_{j-1/2}\big)^2(b(r^n_j) + b(r^n_{j-1}))$

$$(12) \qquad \approx (\frac{\epsilon l(v)}{\Delta y})^2 \times |v_j^{n+1} - v_j^n|^2$$

in deep connection with the CFL restriction.

- Back to the first step

Approximation via relaxation (Suliciu) :

$$
(13)\qquad
\begin{aligned}
&v_t - u_y = 0,\\
&u_t + \Pi_y = 0,\\
&\Pi_t + a^2 u_y = \nu(\mathcal{P}(v, \theta_{y0}) - \Pi),\\
&\theta_t = 0,
\end{aligned}
$$

Proposition 8 *Define :*

$$
\Xi^n_{j-1/2} = \epsilon \frac{L(v_j^{n+1}) - L(v_j^n)}{\Delta t} \quad (\approx \epsilon l(v) u_y),
$$

to get successively

$$
\theta_j^{n+1} = \epsilon \frac{L(v_{j+1}^{n+1}) - L(v_j^{n+1})}{\Delta y} \quad (\approx \epsilon L(v)_y),
$$

$$
\Delta_t(u^2/2 + \mathcal{E}(v) + \tfrac{\theta^2}{2})_j + \tfrac{\Delta t}{\Delta y}\Delta_y(\Pi u + \epsilon\theta l(v) u_y)^n_{j+1/2}
$$

$$
=
$$

$$
\Big\{ - \partial_v p(\bar{v}(v_j^n, v_j^{n+1})) + \big(\tfrac{\epsilon l(v_j^n)}{\Delta y}\big)^2 \times (b(r_j^n) + b(r_{j-1}^n))
$$

$$
-a^2 \Big\} \times |v_j^{n+1} - v_j^n|^2
$$

(14)

Choose consequently a to enforce RHS < 0.

Control The Energy Dissipation Rate

$$a^2 > -\partial_v p(\bar{v}(v_j^n, v_j^{n+1})) + \left(\frac{\epsilon l(v_j^n)}{\Delta y}\right)^2 \times (b(r_j^n) + b(r_{j-1}^n))$$

with $0 \leq b(r) \leq 1$!

In complete agreement with Fourier Analysis :

$$c_{max}^2 = max(-p'(v) + (\frac{\epsilon l(v)}{\Delta y})^2).$$

But in the Elliptic region : $-p'(v) < 0$

$\hookrightarrow$ Excess of Discrete Energy Dissipation

$EDED_j^n :=$

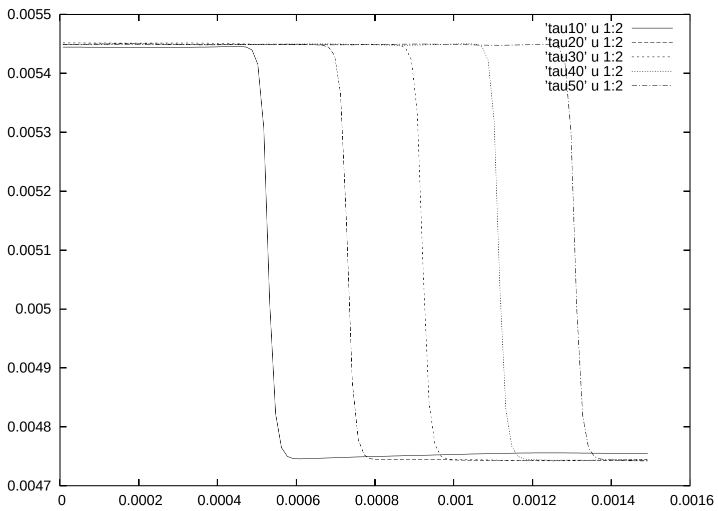
$$\Big\{ -\partial_v p(\bar{v}(v_j^n, v_j^{n+1})) + \big(\tfrac{\epsilon l(v_j^n)}{\Delta y}\big)^2 \times (b(r_j^n) + b(r_{j-1}^n)) - a^2 \Big\} \times |v_j^{n+1} - v_j^n|^2 << 0 \quad \text{in Elliptic region} \tag{15}$$

$\hookrightarrow$ Control the discrete Energy dissipation

Hint : Approximate solutions $\mathbf{v}_{\Delta y}(y, t^n)$

$$\begin{aligned} v_{\Delta y}(y, t^n) &= v_j^n, \quad y \in (y_{j-1/2}, y_{j+1/2}) \\ \theta_{\Delta y}(y, t^n) &= \epsilon(L(v_{j+1}^n) - L(v_j^n))/\Delta y, \\ u_{\Delta y}(y, t^n) &= u_j^n + Du_j^n \times \tfrac{y - y_j}{\Delta y}, \end{aligned} \tag{16}$$

$\hookrightarrow$ Du_j^{n+1} cancels excess of diffusion $EDED_j^n$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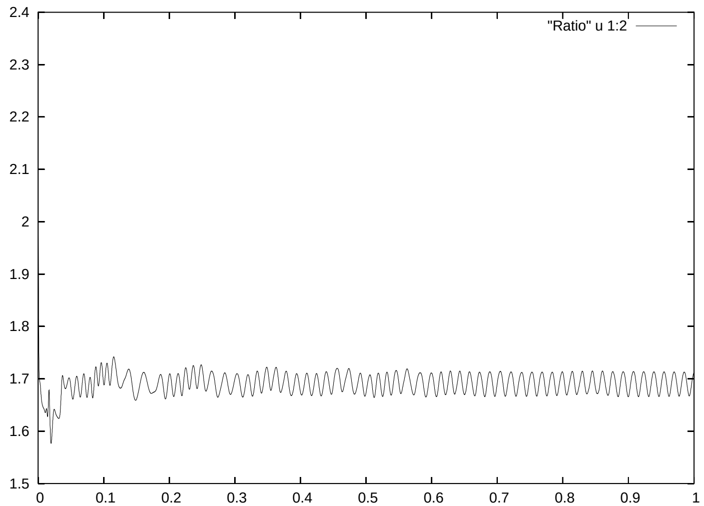
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Explicit Control of Dissipation Rate

- Trivial exact solution with $I\!P^1$ data of :

$$
\begin{aligned}
& v_t - u_y = 0, \\
(17)\quad & u_t + \Pi_y = 0, \qquad (\ (\mu u_y)_y \text{ implicit step}) \\
& \Pi_t + a^2 u_y = 0
\end{aligned}
$$

- First Step : Deduce the first order $EDED$

$$
\begin{aligned}
\Delta_t(u^2/2 + \mathcal{E}(v) + \tfrac{\theta^2}{2})_j &+ \tfrac{\Delta t}{\Delta y}\Delta_y(\Pi u + \epsilon\theta l(v)u_y)^n_{j+1/2} \\
&- \tfrac{\Delta t}{\Delta y}\Delta_y(\mu u u_y)_{j+1/2} + \Delta t\mu(u_y^2)_j \\
&= EDED^n_j \text{ by definition !} \\
&< 0 \text{ with similar choice of a}
\end{aligned}
$$

(18)

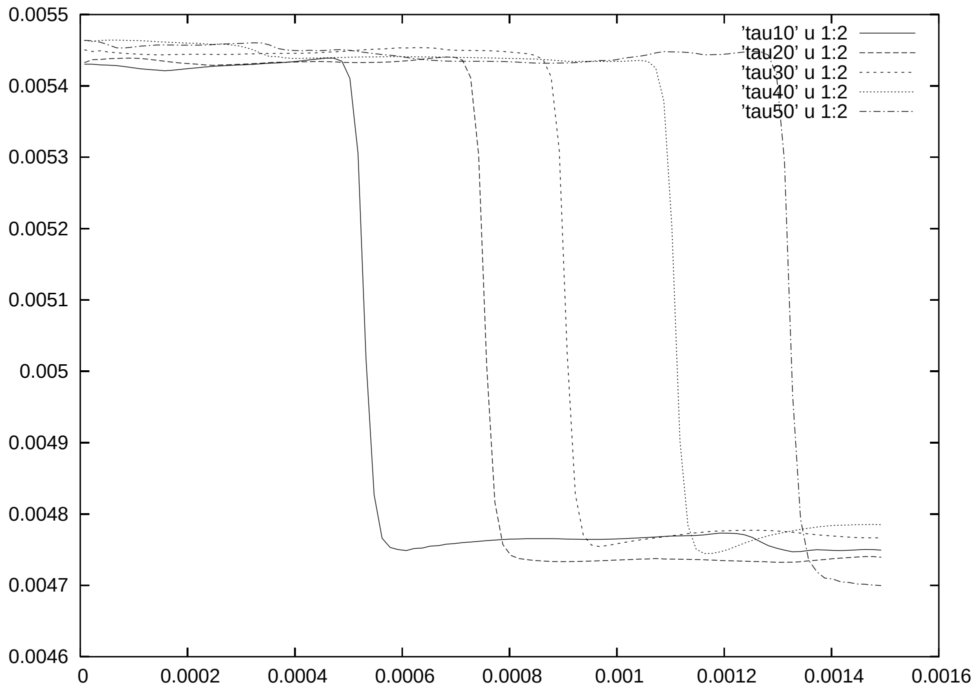
- Second Step : Update the slope

$$
\frac{(Du_j^{n+1})^2}{24} = \frac{(Du_j^n)^2}{24} + \Big\{ -EDED^n_j \Big\}, \qquad (Du\,\Delta_y u)_j \geq 0
$$

to get the corrected Energy dissipation rate

$$
\begin{aligned}
\Delta_t(\textstyle\int u^2/2dy + \mathcal{E}(v) + \tfrac{\theta^2}{2})_j &+ \tfrac{\Delta t}{\Delta y}\Delta_y(\Pi u + \epsilon\theta l(v)u_y) \\
&- \tfrac{\Delta t}{\Delta y}\Delta_y(\mu u u_y)_{j+1/2} + \Delta t\mu(u_y^2)_j = 0
\end{aligned}
$$

(19)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