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- Problems and Perspectives -

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On two fractional step finite volume and finite element schemes for reactive low Mach number flows

Fabrice Babik[*], Thierry Gallouët[**], Jean-Claude Latché[*], Sylvain Suard[*], and Didier Vola[*]

[*] Institut de Radioprotection et de Sûreté Nucléaire, France

[**] Laboratoire d'Analyse, Topologie, Probabilité, UMR 6632, CMI, France

Outline

1. Introduction
2. Finite Volumes formulation
3. Two numerical schemes
4. Numerical tests

Introduction

- **Governing equations:**

$$
\begin{aligned}
&\frac{\partial \varrho}{\partial t} + \nabla \cdot \varrho u = 0 \\
&\frac{\partial \varrho u}{\partial t} + \nabla \cdot (\varrho u \otimes u) = \nabla \cdot \tau - \nabla p + (\rho - \rho_\infty) g \\
&\frac{\partial \varrho z}{\partial t} + \nabla \cdot \varrho z u = \nabla \cdot (\kappa \nabla z) \\
&\varrho = \mathcal{G}(z)
\end{aligned}
$$

+ boundary and initial conditions

- **Several physical problems enter this abstract framework:**
  - Natural convection flows in the low Mach number limit:
    - z stands for the temperature,
    - $\mathcal{G}(z)$ is the equation of state of perfect gaz (at fixed pressure in case of open boundaries; otherwise, the preceding system must be supplemented by an evolution equation for the thermodynamic pressure).
  - Non-premixed laminar flame:
    - z is a Zeldovitch's variable called mixture-fraction,
    - $\mathcal{G}(z)$ derived from $T(z)$, $Y_{\mathrm{F}}(z)$, $Y_{\mathrm{Ox}}(z)$ and $Y_{\mathrm{P}}(z)$.

Particular features and requirements:

- the unknown field z must have convergent and stability properties
  ⇝ construction of a FV numerical scheme which reproduces these features at the discrete level
- $\varrho = \mathcal{G}(z)$: no independant evolution equation can be stated for the fluid density
  ⇝ the mass balance equation acts as a constraint on the velocity
  - use of fractional step schemes, namely projection methods
- FEs for an accurate velocity and pressure computation
  - nonconforming velocity approximations (dof located at the center of the faces) for a coupling with a FV method for the advection-diffusion of z

- Overshoots or undershoots (even small) have a dramatic effect in chemically reacting flows
- From both a physical and numerical viewpoint, all the species concentrations remain positive

A maximum principle stands for the unknown field z

- As the velocity is not divergence free, the conservation equation for z does not imply any maximum principle...
- But it can be combined with the mass balance equation as follows:

$$\frac{\partial \varrho z}{\partial t} + \nabla \cdot \varrho z u = \varrho(\frac{\partial z}{\partial t} + u \cdot \nabla z) + z \underbrace{(\frac{\partial \varrho}{\partial t} + \nabla \cdot \varrho u)}_{=0} = \nabla \cdot (\kappa \nabla z)$$

For this latter equation, if $z(x,0) \in [0,1]$ and z takes values in $[0,1]$ on Dirichlet boundaries, then $z(x,t) \in [0,1], \ \forall x, \ \forall t$.

Mixed FV / FE formulation

1. Introduction
2. Finite Volumes formulation
   - 2.1 A finite volumes scheme for the transport of z
   - 2.2 High order interpolation FV schemes
3. Two numerical schemes
4. Numerical tests

2.1 A finite volumes scheme for the transport of z (1/4)

- Definition: M is a M-matrix if

$$\begin{cases} M_{ii} > 0, & 1 \leq i \leq N, \\ M_{ij} \leq 0, & \text{for } i \neq j \\ M_{ii} - \sum_{j \neq i} |M_{ij}| \geq 0, & \forall i \\ M_{ii} - \sum_{j \neq i} |M_{ij}| > 0, & \text{for one node} \end{cases}$$

- If M is a M-matrix: if $M\mathbf{X} \geq 0, \implies \mathbf{X} \geq 0$

- If M^t is an M-matrix, $M\mathbf{X} \geq 0 \implies X \geq 0$

- Scheme: solve in sequence a prediction for the density, then the (now linear) convection-diffusion equation for z, and, finally, update the density using the constitutive equation.

$$\left|\begin{array}{l} m_K \dfrac{\tilde{\varrho}_K - \varrho_K^n}{k} + \displaystyle\sum_{\sigma \in \mathcal{E}_K} m_\sigma \, v_\sigma \, \tilde{\varrho}_\sigma = 0 \\ m_K \dfrac{\tilde{\varrho}_K \, z_K^{n+1} - \varrho_K^n \, z_K^n}{k} + \displaystyle\sum_{\sigma \in \mathcal{E}_K} m_\sigma \, v_\sigma \, \tilde{\varrho}_\sigma \, z_\sigma^{n+1} + \displaystyle\sum_{\sigma \in \mathcal{E}_K} \dfrac{m_\sigma}{d_\sigma} \kappa \, (z_K^{n+1} - z_L^{n+1}) = 0 \\ \varrho_K^{n+1} = \mathcal{G}(z_K^{n+1}) \end{array}\right.$$

where :

- v_σ stands for the normal velocity to the edge σ
- $\tilde{\varrho}_\sigma$ and z_σ^{n+1} stand for the standard upwind approximation for $\tilde{\varrho}$ and z^{n+1}.

- Of course, the prediction step makes sense only if the mass balance holds.

Exemple: see the full scheme hereafter.

2.1 A finite volumes scheme for the transport of z (3/4)

- The discrete operator associated to the first equation is the transposed of an M-matrix.
- The discrete operator associated to the second equation is an M-matrix:

$$\Sigma = \sum_L A_{K,L} = m_K \frac{\tilde{\varrho}_K}{k} + \sum_{\sigma \in \mathcal{E}_K} m_\sigma v_{\sigma,K} \tilde{\varrho}_\sigma = m_K \frac{\varrho_K^n}{k} > 0$$

- Let $\overline{z}^n$ and $\underline{z}^n$ be defined by $\overline{z}^n = \max_K z_K^n$, $\underline{z}^n = \min_K z_K^n$. Then:

$$\forall K, \qquad z_K^{n+1} \in [\underline{z}^n, \overline{z}^n]$$

Idea of the proof:

$$m_K \frac{\tilde{\varrho}_K (z_K^{n+1} - \overline{z}^n)}{k} + \sum_{\sigma \in \mathcal{E}_K} m_\sigma \, v_\sigma \, \tilde{\varrho}_\sigma \, (z_\sigma^{n+1} - \overline{z}^n)$$
$$+ \sum_{\sigma \in \mathcal{E}_K} \frac{m_\sigma}{d_\sigma} \kappa \left[(z_K^{n+1} - \overline{z}^n) - (z_L^{n+1} - \overline{z}^n) \right] = m_K \frac{\varrho_K^n z_K^n}{k} - \Sigma \, \overline{z}^n$$
$$= \underbrace{m_K \frac{\varrho_K^n (z_K^n - \overline{z}^n)}{k}}_{\leq 0}$$

☐ A L^2 stability property.

Multiplying by z the advection-diffusion equation for z and integrating over Ω yields:

$$\int_\Omega \left[\frac{\partial \varrho z}{\partial t} + \nabla \cdot (\varrho z u)\right] z = \int_\Omega [\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho u)]\ z^2 + \int_\Omega \varrho z \frac{\partial z}{\partial t} + \varrho z u \cdot \nabla z$$

$$= \frac{1}{2} \int_\Omega \varrho \frac{\partial z^2}{\partial t} + \varrho u \cdot \nabla (z^2) \qquad \text{(mass balance equation)}$$

$$= \frac{1}{2} \int_\Omega \varrho \frac{\partial z^2}{\partial t} - z^2 \nabla \cdot (\varrho u) \qquad \text{(integration by parts)}$$

$$= \frac{1}{2} \int_\Omega \varrho \frac{\partial z^2}{\partial t} + z^2 \frac{\partial \varrho}{\partial t} \qquad \text{(mass balance equation)}$$

$$= \frac{1}{2} \frac{\partial}{\partial t} \int_\Omega \varrho z^2 = - \int_\Omega \kappa |\nabla z|^2$$

The same computation can be followed "line by line" in the discrete case, which provides:

- a stability result,
- a tool for proving an error estimate ?

2.2 High order interpolation FV schemes

☐ **A second order FV scheme for diffusive cases:**

- Numerical experiments show that the spatial accuracy is limited to first order as soon as an upwind discretization is used for the prediction of the density.

- Use of a centered deferred correction scheme (2^{nd} order):

$$\frac{\tilde{\rho} - \rho^n}{\Delta t} + \nabla_{\mathrm{U}} \cdot (\rho v)^{n+1} + \beta \left(\nabla_{\mathrm{C}} \cdot (\rho v)^n + \nabla_{\mathrm{U}} \cdot (\rho v)^n \right) = 0$$

The β parameter is chosen to ensure that $\tilde{\rho}$ remains positive.

- Use of an hybrid FV interpolation scheme for the transport of z

$$\frac{\partial \varrho z}{\partial t} + \nabla_{\mathrm{H}}.(\varrho z u) = \nabla \cdot (\kappa \nabla z) \quad \text{with } \nabla_{\mathrm{H}}.(\phi) = \alpha \nabla_{\mathrm{C}}.(\phi) + (1-\alpha) \nabla_{\mathrm{U}}.(\phi), \ \alpha \in [0,1]$$

Two numerical schemes

3.1 A non-conservative scheme

solve for $\tilde{\varrho}$ $$\frac{\tilde{\varrho} - \varrho^n}{\Delta t} + \nabla_{\mathrm{U}} \cdot \tilde{\varrho} u^n = 0$$

solve for z^{n+1} $$\frac{\tilde{\varrho} z^{n+1} - \varrho^n z^n}{\Delta t} + \nabla_{\mathrm{U}} \cdot \tilde{\varrho} z^{n+1} u^n - \Delta_{\mathrm{C},\kappa}\, z^{n+1} = 0$$

ϱ^{n+1} given by $$\varrho^{n+1} = \mathcal{G}(z^{n+1})$$

solve for $\tilde{u}$ $$\frac{\tilde{\varrho}\tilde{u} - \varrho^n u^n}{\Delta t} + \nabla \cdot (\tilde{\varrho} u^n \otimes \tilde{u}) - \nabla \cdot \tau(\tilde{u}) + \nabla p^n = g^{n+1}$$

solve for $p^{n+1},\ u^{n+1}$ $$\left| \begin{array}{l} \dfrac{\varrho^{n+1} u^{n+1} - \tilde{\varrho}\tilde{u}}{\Delta t} + \nabla (p^{n+1} - p^n) = 0 \\ \nabla \cdot \varrho^{n+1} u^{n+1} = -\dfrac{\varrho^{n+1} - \varrho^n}{\Delta t} \end{array} \right.$$

- the density is updated after the computation of z^{n+1}
- this scheme does not conserve the quantity ϱz

3.2 A conservative scheme

solve for $\tilde{\varrho}$ $$\frac{\tilde{\varrho} - \varrho^n}{\Delta t} + \nabla_{\mathrm{U}} \cdot \tilde{\varrho} u^n = 0$$

solve for $\tilde{z}$ $$\frac{\tilde{\varrho}\tilde{z} - \varrho^n z^n}{\Delta t} + \nabla_{\mathrm{U}} \cdot \tilde{\varrho}\tilde{z} u^n - \Delta_{\mathrm{C},\kappa}\, \tilde{z} = 0$$

ϱ^{n+1} given by $$\varrho^{n+1} = \mathcal{G}(\tilde{z})$$

solve for $\tilde{u}$ $$\frac{\tilde{\varrho}\tilde{u} - \varrho^n u^n}{\Delta t} + \nabla \cdot (\tilde{\varrho} u^n \otimes \tilde{u}) - \nabla \cdot \tau(\tilde{u}) + \nabla p^n = g^{n+1}$$

solve for $p^{n+1},\ u^{n+1}$ $$\left| \begin{array}{l} \dfrac{\varrho^{n+1} u^{n+1} - \tilde{\varrho}\tilde{u}}{\Delta t} + \nabla (p^{n+1} - p^n) = 0 \\ \nabla \cdot \varrho^{n+1} u^{n+1} = -\dfrac{\varrho^{n+1} - \varrho^n}{\Delta t} \end{array} \right.$$

solve for z^{n+1} $$\frac{\varrho^{n+1} z^{n+1} - \varrho^n z^n}{\Delta t} + \nabla_{\mathrm{CU}} \cdot \varrho^{n+1} z^{n+1} u^{n+1} - \Delta_{\mathrm{C},\kappa}\, z^{n+1} = 0$$

- stability of the last step requires:
  - a centered approximation for the density
  - an upwind approximation for the variable z

Numerical tests

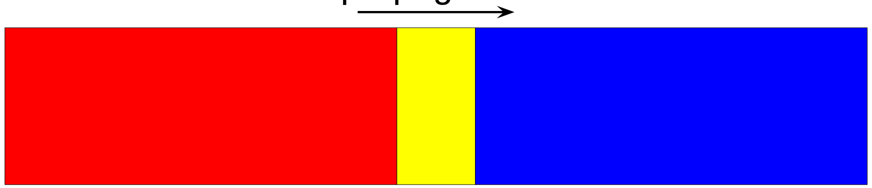
4.1 Analytical premixed flame propagation (1/2)

- **Governing equations:**

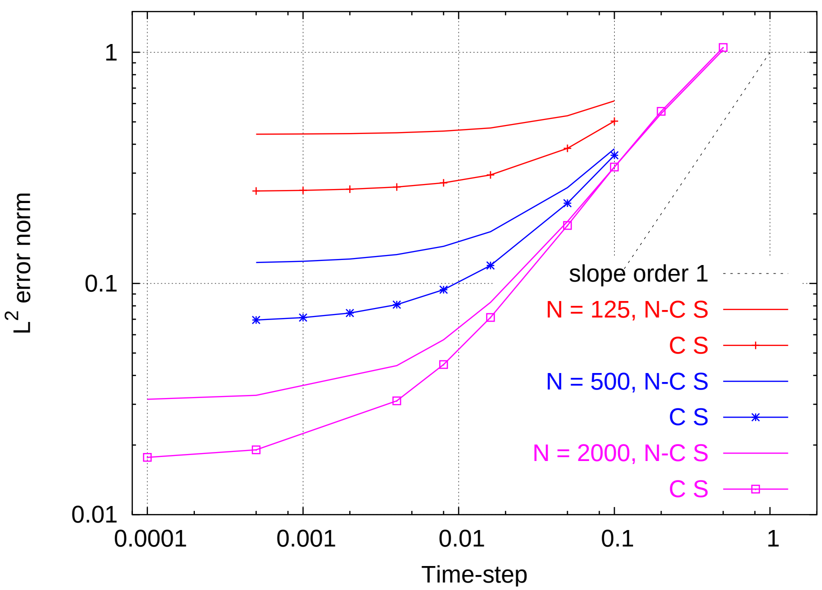
$$\frac{\partial \varrho}{\partial t} + \nabla \cdot \varrho u = 0$$
$$\frac{\partial \varrho u}{\partial t} + \nabla \cdot (\varrho u \otimes u) = \nabla \cdot \tau - \nabla p$$
$$\frac{\partial \varrho z}{\partial t} + \nabla \cdot \varrho z u = \nabla \cdot (\kappa \nabla z) + f(z)$$
$$\varrho = 1/(1 - \gamma + \gamma z)$$

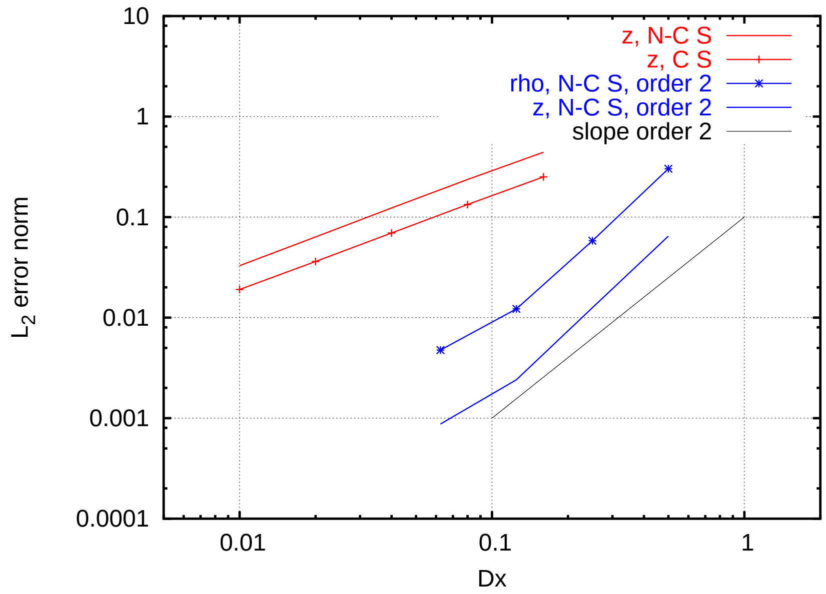
- **Analytical solution:**

$$z(x,t) = \frac{1}{2}\left(1 - \tanh\left[\frac{x - ut}{\delta}\right]\right)$$



4.1 Analytical premixed flame propagation (2/2)

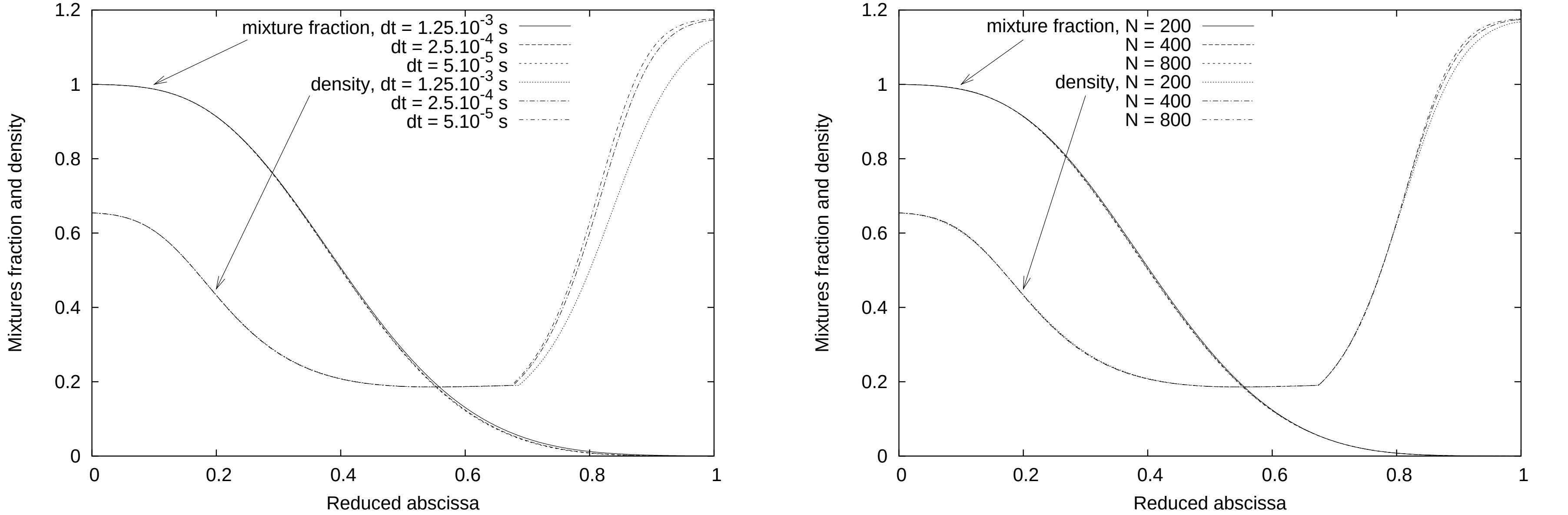




L^2 error norm obtained with the non-conservative (N-C S) and conservative scheme (C S), as a function of: left: time-step for differents grid size; right: grid size for a time-step of 5.10^{-4}.

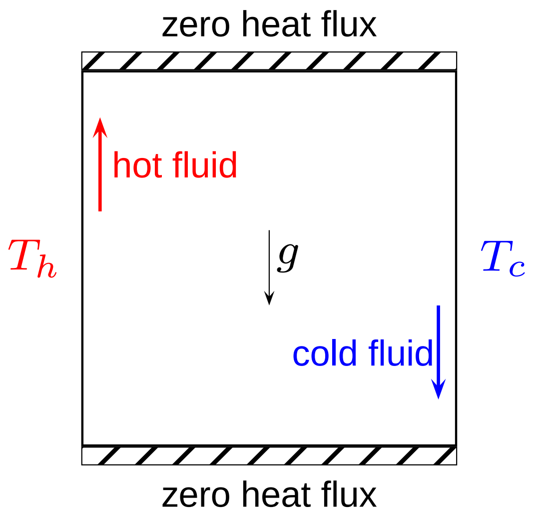
4.2 Planar non-premixed flame propagation

- Infinitely fast chemistry assumption: Burke-Schumann approximation
- The variable z stands for the mixture fraction
- A very stiff problem: Large gradients of density and temperature appear near $z_S \approx 0.05$



Distributions of mixture fraction and density along the flow direction obtained with the non-conservative scheme for three time steps (left) and three mesh sizes (right).

- A buoyancy-driven flow in a two-dimensional square enclosure [0,L] $\times$ [0,L] with large temperature differences
- Two insulated walls and two vertical walls heated to T_h respectively cooled down to T_c.



- Flow specification:

Dimension	2D
Geometry	Cartesian
Temporal	Steady
	laminar & Thermal
Gas law	Perfect gas

- Nusselt number:

$$Nu(y) = \frac{L}{k_0(T_h - T_c)} k \frac{\partial T}{\partial x}\Big|_w$$

- Average Nusselt number:

$$\langle Nu \rangle = \frac{1}{L} \int_{y=0}^{y=L} Nu(y)\, dy,$$

$$\langle Nu \rangle_h + \langle Nu \rangle_c = 0$$

- Governing equations:

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot \varrho u = 0$$

$$\frac{\partial \varrho u}{\partial t} + \nabla \cdot (\varrho u \otimes u) = \nabla \cdot \tau - \nabla p + (\rho - \rho_\infty) g$$

$$\frac{\partial \varrho h}{\partial t} + \nabla \cdot \varrho h u = \nabla \cdot (\kappa \nabla h) + \frac{dP}{dt}$$

$$P = \varrho R T$$

- Test case T2 (H. Paillère and P. Le Quéré):
  - $Ra = Pr \dfrac{g\,\rho_0^2\,(T_h - T_c)\,L^3}{T_0 \mu_0^2} = 10^6$, Sutherland's Law, $\epsilon = \dfrac{T_h - T_c}{T_h + T_c} = 0.6$

- Initial conditions: The problem is completely defined by the Rayleigh number, the value of ϵ and the following coefficient:
  - $P_0 = 101325$ Pa, $T_0 = 600$ K, $\rho_0 = P_0/(RT_0)$,
  - $Pr = 0.71$, $\gamma = 1.4$, $g = 9.81$ m/s^2

- Boundary conditions:
  - hot wall: $T_h = T_0(1+\epsilon)$, cold wall: $T_c = T_0(1-\epsilon)$
  - horizontal walls: adiabatic conditions, all walls: no-slip condition for the velocity

	Ref.	20 × 20	40 × 40	80 × 80	120 × 120	160 × 160
relative error	0	0.095 0.	0.075 0.	0.044 0.	0.031	0.023
Nu_h	8.686	7.889 7.353	8.408 8.131	8.389 8.372	8.386	8.397

- $e := 1 + \langle Nu \rangle_c / \langle Nu \rangle_h \propto O(h)$ for scheme 1