Introduction to cell-centered Lagrangian schemes

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September 13th, 2017



- Introduction
- Gas dynamics system of equations
- First-order numerical scheme for the 2D gas dynamics
- 4 High-order extension in the 2D case
- Numerical results in 2D

Eulerian formalism (spatial description)

- fixed referential attached to the observer
- fixed observation zone through the fluid flows

Lagrangian formalism (material description)

- moving referential attached to the material
- observation zone moved and deformed as the fluid flows

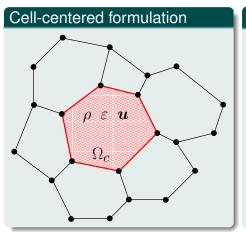
Lagrangian formalism advantages

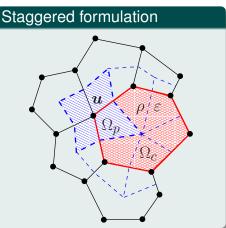
- adapted to problems undergoing large deformations
- naturally tracks interfaces in multi-material flows
- avoids the numerical diffusion of the convection terms

Lagrangian formalism drawbacks

- Robustness issue in the case of strong vorticity or shear flows
 - ALE method (Arbitrary Lagrangian-Eulerian)

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Definitions

- \bullet ρ the fluid density
- u the fluid velocity
- e the fluid specific total energy
- p the fluid pressure
- $\varepsilon = e \frac{1}{2} u^2$ the fluid specific internal energy

Euler equations

$$\bullet \ \frac{\partial \rho}{\partial t} + \nabla_{x} \cdot \rho \, \boldsymbol{u} = 0$$

$$\bullet \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla_{x} \cdot (\rho \mathbf{u} \otimes \mathbf{u} + \rho \mathbf{I}_{d}) = \mathbf{0}$$

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ho \, oldsymbol{e}}{\partial t} +
abla_{\!\scriptscriptstyle X} \, . \, (
ho \, oldsymbol{u} \, oldsymbol{e} +
ho \, oldsymbol{u}) = 0$$

Thermodynamical closure

• $p = p(\rho, \varepsilon)$

Equation of state

Moving referential

- X is the position of a point of the fluid in its initial configuration
- $\mathbf{x}(\mathbf{X},t)$ is the actual position of this point, moved by the fluid flow

Trajectory equation

•
$$x(X,0) = X$$

Material derivative

- $f(\mathbf{x}, t)$ is a smooth fluid variable
- $\bullet \frac{\mathrm{d} f(\boldsymbol{x},t)}{\mathrm{d} t} = \frac{\partial f(\boldsymbol{x},t)}{\partial t} + \boldsymbol{u} \cdot \nabla_{\boldsymbol{x}} f(\boldsymbol{x},t)$



Definitions

- $au = \frac{1}{
 ho}$ the specific volume
- $U = (\tau, \boldsymbol{u}, \boldsymbol{e})^{t}$ the solution vector
- $F(U) = (-u, 1(1) p, 1(2) p, 1(3) p, p u)^t$ where $1(i) = (\delta_{i1}, \delta_{i2}, \delta_{i3})^t$
- $a = a(\rho, \varepsilon)$ the sound speed

Updated Lagrangian formulation

Moving configuration

Non-conservative formulation

•
$$\rho \frac{\mathrm{d} U}{\mathrm{d} t} + \mathsf{A}_x(\mathsf{U}) \frac{\partial U}{\partial x} + \mathsf{A}_y(\mathsf{U}) \frac{\partial U}{\partial y} + \mathsf{A}_z(\mathsf{U}) \frac{\partial U}{\partial z} = 0$$

- $A_n = A_x n_x + A_y n_y + A_z n_z$ with **n** a unit vector
- $\lambda(U) = \{-\rho a, 0, \rho a\}$ the eigenvalues of $A_n(U)$

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Deformation gradient tensor

- \bullet J = $\nabla_X x$
- $|J| = \det J > 0$
- ullet $\nabla_X \cdot \left(|\mathsf{J}| \mathsf{J}^{-\mathsf{t}} \right) = \mathbf{0}$

Jacobian of the fluid flow Positive control volume Piola compatibility condition

Mass conservation

- $\bullet \int_{\omega(0)} \rho^0 \, \mathrm{d}V = \int_{\omega(t)} \rho \, \mathrm{d}V$
- $\bullet \int_{\omega(t)} \rho \, \mathrm{d} v = \int_{\omega(0)} \rho \, |\mathsf{J}| \, \mathrm{d} V$

Total Lagrangian formulation

Fixed configuration

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Définitions

- $0 = t^0 < t^1 < \cdots < t^N = T$ a partition of the time domain [0, T]
- $\omega^0 = \bigcup_{c=1,I} \omega_c^0$ a partition of the initial domain ω^0
- ω_c^n the image of ω_c^0 at time t^n through the fluid flow
- m_c the constant mass of cell ω_c
- $U_c^n = (\tau_c^n, u_c^n, e_c^n)^t$ the discrete solution

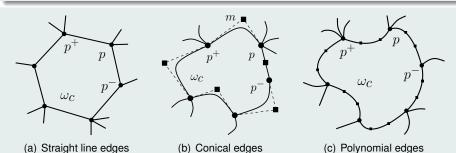


Figure: Generic polygonal cell

Integration

•
$$U_c^{n+1} = U_c^n - \frac{\Delta t^n}{m_c} \int_{\partial \omega_c} \overline{F} \cdot \boldsymbol{n} \, ds$$

Integration of the cell boundary term (analytically, quadrature, ...)

General first-order finite volumes scheme

$$\bullet \ \mathsf{U}_c^{n+1} = \mathsf{U}_c^n - \frac{\Delta t^n}{m_c} \sum_{q \in \mathcal{Q}_c} \overline{\mathsf{F}}_{qc} \cdot \mathit{I}_{qc} \boldsymbol{n}_{qc}$$

- $\overline{\mathsf{F}}_{qc} = (-\overline{\pmb{u}}_q, \ \mathbb{1}(1)\,\overline{p}_{qc}, \ \mathbb{1}(2)\,\overline{p}_{qc}, \ \overline{p}_{qc}\,\overline{\pmb{u}}_q)^{\mathsf{t}}$ numarical flux at point q

Definitions

- Q_c the chosen control point set of cell ω_c
- Iac nac some normals to be defined



Remark

- \overline{F}_{qc} is local to the cell ω_c
- ullet Only $\overline{oldsymbol{u}}_{qc}=\overline{oldsymbol{u}}_q$ needs to be continuous, to advect the mesh
- Loss of the scheme conservation?

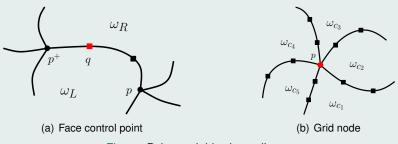


Figure: Points neighboring cell sets

1D numerical fluxes

- ullet $\overline{
 ho}_{qc}=
 ho_c^n-\widetilde{z}_{qc}\left(\overline{m{u}}_q-m{u}_c^n
 ight)$. $m{n}_{qc}$
- $\tilde{z}_{ac} > 0$ local approximation of the acoustic impedance

Conservation

•
$$\sum_{c} m_c U_c^{n+1} = \sum_{c} m_c U_c^n + BC$$
 ?

- ullet For sake of simplicity, we consider BC = 0
- ullet Necessary condition: $\sum_{c}\sum_{q\in\mathcal{Q}_{c}}\overline{p}_{qc}\,l_{qc}oldsymbol{n}_{qc}=oldsymbol{0}$

Example of a solver: LCCDG schemes

- Conditions suffisantes
- $\bullet \ \, \forall p \in \mathcal{P}(\omega), \quad \sum_{c \in \mathcal{C}_p} \left[\overline{p}_{pc}^- \, l_{pc}^- \, n_{pc}^- + \overline{p}_{pc}^+ \, l_{pc}^+ \, n_{pc}^+ \right] = \mathbf{0}$

$$\implies \quad \overline{\boldsymbol{u}}_{\rho} = \Big(\sum_{c \in \mathcal{C}_{\rho}} \mathsf{M}_{\rho c}\Big)^{-1} \sum_{c \in \mathcal{C}_{\rho}} \Big(\mathsf{M}_{\rho c} \boldsymbol{u}_{c}^{n} + \rho_{c}^{n} I_{\rho c} \boldsymbol{n}_{\rho c}\Big)$$

- $\bullet \ \, \forall q \in \mathcal{Q}(\omega) \setminus \mathcal{P}(\omega), \quad (\overline{\rho}_{qL} \overline{\rho}_{qR}) \, \textit{I}_{qL} \textbf{\textit{n}}_{qL} = \textbf{\textit{0}} \quad \Longleftrightarrow \quad \overline{\rho}_{qL} = \overline{\rho}_{qR}$
 - $\implies \quad \overline{\boldsymbol{u}}_{q} = \left(\frac{\widetilde{\boldsymbol{z}}_{qL}\,\boldsymbol{u}_{L}^{n} + \widetilde{\boldsymbol{z}}_{qR}\,\boldsymbol{u}_{R}^{n}}{\widetilde{\boldsymbol{z}}_{qL} + \widetilde{\boldsymbol{z}}_{qR}}\right) \frac{\boldsymbol{p}_{R}^{n} \boldsymbol{p}_{L}^{n}}{\widetilde{\boldsymbol{z}}_{qL} + \widetilde{\boldsymbol{z}}_{qR}}\,\,\boldsymbol{n}_{qf_{pp^{+}}}$

Convex combinaison

$$\bullet \ \mathsf{U}_c^{n+1} = \mathsf{U}_c^n - \frac{\Delta t^n}{m_c} \sum_{q \in \mathcal{Q}_c} \overline{\mathsf{F}}_{qc} \cdot \mathsf{I}_{qc} \mathbf{n}_{qc} + \frac{\Delta t^n}{m_c} \mathsf{F}(\mathsf{U}_c^n) \cdot \underbrace{\sum_{q \in \mathcal{Q}_c} \mathsf{I}_{qc} \mathbf{n}_{qc}}_{=\mathbf{0}}$$

•
$$U_c^{n+1} = (1 - \lambda_c) U_c^n + \sum_{q \in \mathcal{Q}_c} \lambda_{qc} \overline{U}_{qc}$$

Definitions

•
$$\lambda_{qc} = \frac{\Delta t^n}{m_c} \widetilde{z}_{qc} I_{qc}$$
 and $\lambda_c = \sum_{q \in \mathcal{Q}_c} \lambda_{qc}$

•
$$\overline{\mathsf{U}}_{qc} = \mathsf{U}_c^n - \frac{\left(\overline{\mathsf{F}}_{qc} - \mathsf{F}(\mathsf{U}_c^n)\right)}{\widetilde{z}_{qc}}$$
 . n_{qc}

CFL condition

Semi-discret first-order scheme

•
$$m_c \frac{\mathrm{d} U_c}{\mathrm{d} t} = -\sum_{q \in \mathcal{Q}_c} \overline{\mathsf{F}}_{qc} \cdot I_{qc} n_{qc}$$

Gibbs identity

• $T dS = d\varepsilon + p d\tau = de - u \cdot du + p d\tau$

Semi-discret production of entropy

$$\bullet \ m_c \, T_c \frac{\mathrm{d} \, S_c}{\mathrm{d} t} = m_c \frac{\mathrm{d} \, e_c}{\mathrm{d} t} + \boldsymbol{u}_c \cdot m_c \frac{\mathrm{d} \, \boldsymbol{u}_c}{\mathrm{d} t} + p_c \, m_c \frac{\mathrm{d} \, \tau_c}{\mathrm{d} t}$$

$$\bullet \ m_c \, T_c \frac{\mathrm{d} \, S_c}{\mathrm{d} t} = \sum_{q \in \mathcal{Q}_c} \widetilde{z}_{qc} \, I_{qc} \left[(\overline{\boldsymbol{u}}_q - \boldsymbol{u}_c) \cdot \boldsymbol{n}_{qc} \right]^2 \ge 0$$

Positivity of the discrete scheme



F. VILAR, C.-W. SHU AND P.-H. MAIRE, *Positivity-preserving* cell-centered Lagrangian schemes for multi-material compressible flows: Form first-order to high-orders. Part II: The 2D case. JCP, 2016.

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High-order extension of the finite-volume scheme

MUSCL, (W)ENO, DG, ...

Mean values equation

•
$$\mathsf{U}_c^{n+1} = \mathsf{U}_c^n - \frac{\Delta t^n}{m_c} \sum_{q \in \mathcal{Q}_c} \overline{\mathsf{F}}_{qc} \cdot l_{qc} n_{qc}$$

• In $\overline{\mathsf{F}}_{qc}$, the mean values are substituted by the high-order values U_{qc} in ω_c at points q

Updated or total Lagrangian formulation

$$\qquad \rho \, \frac{\mathrm{d} \, \mathsf{U}}{\mathrm{d} t} + \nabla_{\mathsf{X}} \, \boldsymbol{\cdot} \, \mathsf{F}(\mathsf{U}) = 0 \qquad \text{ou} \qquad \rho^0 \frac{\mathrm{d} \, \mathsf{U}}{\mathrm{d} t} + \nabla_{\mathsf{X}} \, \boldsymbol{\cdot} \, \big(|\mathsf{J}| \mathsf{J}^{-1} \mathsf{F}(\mathsf{U}) \big) = 0$$

Piecewise polynomial approximation

- $\mathsf{U}^n_{h,c}(\mathbf{x})$ the polynomial approximation of the solution on ω^n_c
- $\mathsf{U}^n_{h,c}(\mathbf{X})$ the polynomial approximation of the solution on ω^0_c
- ullet $U_{qc}=U_{h,c}^n(extbf{ ilde{x}}_q)$ (moving config.) or $U_{qc}=U_{h,c}^n(extbf{ ilde{x}}_q)$ (fixed config.)

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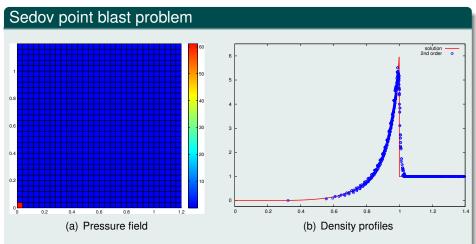
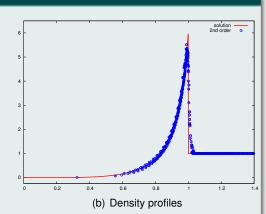


Figure : Solution at time t=1 for a Sedov problem on a 30 \times 30 Cartesian mesh

Sedov point blast problem



(a) Pressure field

Figure : Solution at time t = 1 for a Sedov problem on a 30 \times 30 Cartesian mesh

Sedov point blast problem

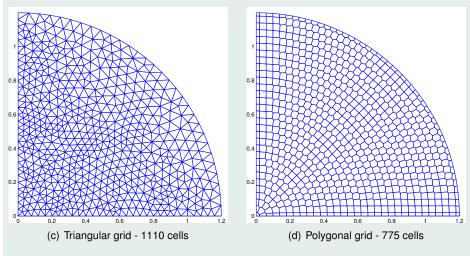


Figure: Initial unstructured grids for Sedov point blast problem

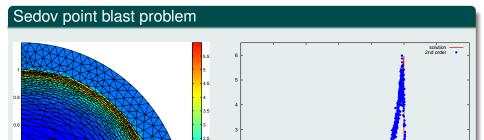


Figure : Solution at time t = 1 for a Sedov problem on a grid made of 1110 triangular cells

0.2

0.4

0.8

(f) Density profiles

(e) Density field

0.4

0.2

1.2

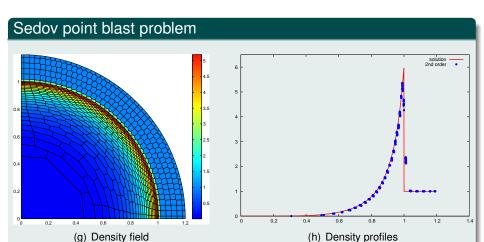


Figure : Solution at time t = 1 for a Sedov problem on a grid made of 775 polygonal cells

Underwater TNT explosion

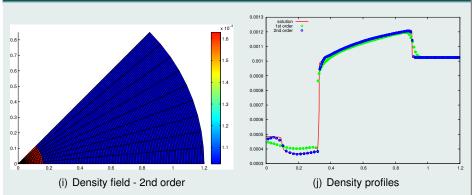
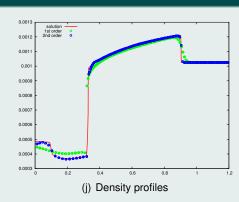


Figure : Solution at time $t = 2.5 \times 10^{-4}$ for a underwater TNT explosion on a 120×9 polar mesh

Underwater TNT explosion



(i) Density field - 2nd order

Figure : Solution at time $t = 2.5 \times 10^{-4}$ for a underwater TNT explosion on a 120×9 polar mesh

Aluminium projectile impact problem

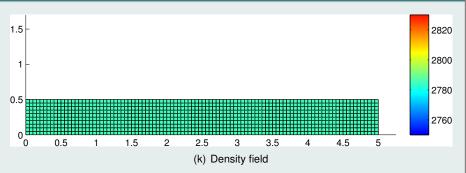


Figure : Solution at time t = 0.05 for a projectile impact problem on a 100×10 Cartesian mesh

Aluminium projectile impact problem

(k) Density field

Figure : Solution at time t = 0.05 for a projectile impact problem on a 100×10 Cartesian mesh

Taylor-Green vortex

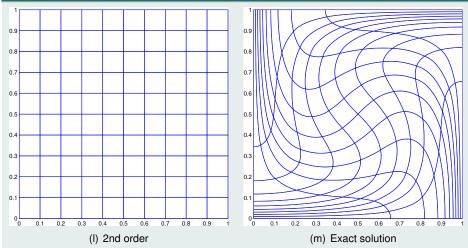
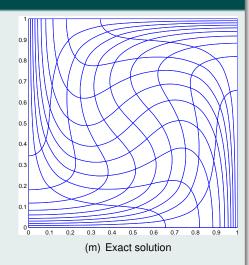


Figure : Final deformed grids at time t = 0.75, on a 10 \times 10 Cartesian mesh

Taylor-Green vortex



(I) 2nd order

Figure : Final deformed grids at time t = 0.75, on a 10 \times 10 Cartesian mesh

Convergence rates

	L ₁		L ₂		L_{∞}	
h	$E_{L_1}^h$	$q_{L_1}^h$	$E_{L_2}^h$	$q_{L_2}^h$	$E_{L_{\infty}}^{h}$	$q_{L_{\infty}}^{h}$
1/10	5.06E-3	1.94	6.16E-3	1.93	2.20E-2	1.84
10 1 20	1.32E-3	1.98	1.62E-3	1.97	5.91E-3	1.95
$\frac{1}{40}$	3.33E-4	1.99	4.12E-4	1.99	1.53E-3	1.98
1 80	8.35E-5	2.00	1.04E-4	2.00	3.86E-4	1.99
160	2.09E-5	-	2.60E-5	-	9.69E-5	-

Table: Convergence rates on the pressure for a 2nd order DG scheme

Taylor-Green vortex

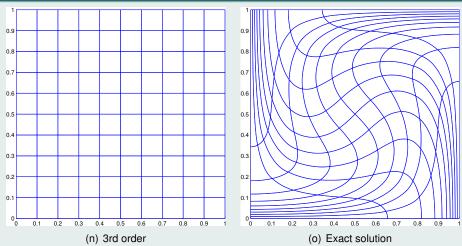
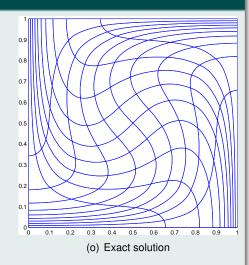


Figure : Final deformed grids at time t = 0.75, on a 10 \times 10 Cartesian mesh

Taylor-Green vortex



(n) 3rd order

Figure : Final deformed grids at time t = 0.75, on a 10 \times 10 Cartesian mesh

Convergence rates

	L_1		L ₂		L_{∞}	
h	$E_{L_1}^h$	$q_{L_1}^h$	$E_{L_2}^h$	$q_{L_2}^h$	$E_{L_{\infty}}^{h}$	$q_{L_{\infty}}^{h}$
1/10	2.67E-4	2.96	3.36E-7	2.94	1.21E-3	2.86
<u>1</u> 20	3.43E-5	2.97	4.36E-5	2.96	1.66E-4	2.93
$\frac{1}{40}$	4.37E-6	2.99	5.59E-6	2.98	2.18E-5	2.96
<u>1</u>	5.50E-7	2.99	7.06E-7	2.99	2.80E-6	2.99
160	6.91E-8	-	8.87E-8	-	3.53E-7	-

Table: Convergence rates on the pressure for a 3rd order DG scheme

Polar meshes - symmetry preservation

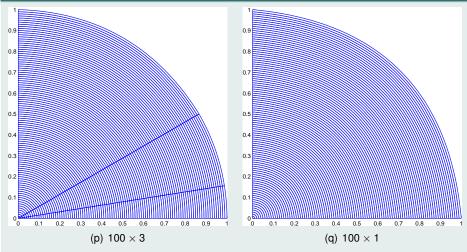


Figure: Curvilinear grids defined in polar coordinates

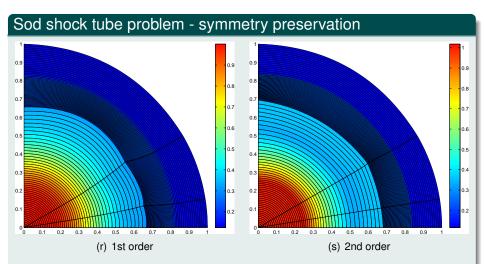


Figure: Density fields with 1st and 2nd order schemes on a 3rd mesh

Sod shock tube problem - symmetry preservation

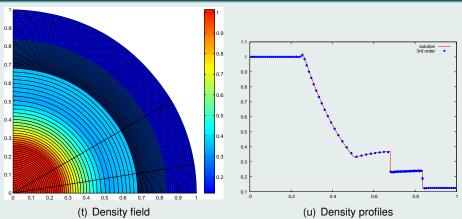


Figure : 3rd order solution for a Sod shock tube problem on a 100 \times 3 polar grid

Sod shock tube problem - symmetry preservation

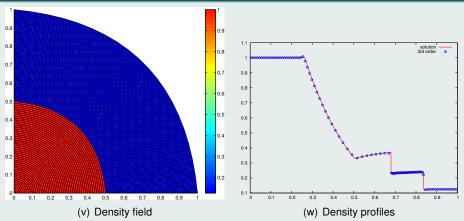
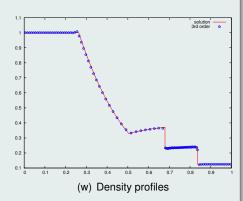


Figure : 3rd order solution for a Sod shock tube problem on a 100 \times 1 polar grid

Sod shock tube problem - symmetry preservation



(v) Density field

Figure : 3rd order solution for a Sod shock tube problem on a 100 \times 1 polar grid

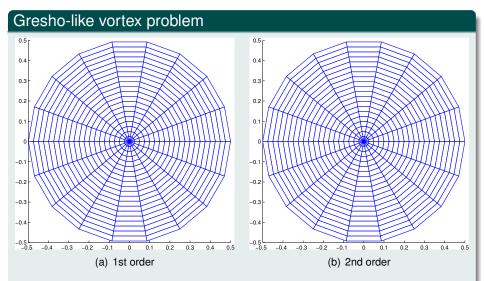


Figure : Final deformed grids at time t = 1, on a 20 \times 18 polar mesh

Gresho-like vortex problem

(a) 1st order

(b) 2nd order

Figure : Final deformed grids at time t = 1, on a 20 \times 18 polar mesh

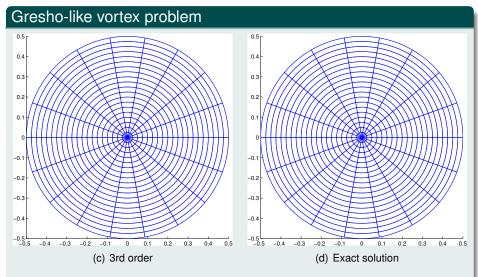


Figure: Final deformed grids at time t = 1, on a 20 \times 18 polar mesh

Gresho-like vortex problem

(c) 3rd order

(d) Exact solution

Figure : Final deformed grids at time t = 1, on a 20 \times 18 polar mesh



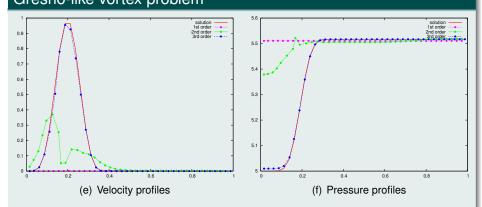


Figure : Velocity and pressure profiles at time t=1, on a 20 imes 18 polar grid

Gresho-like vortex problem

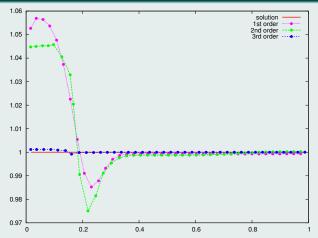


Figure : Density profiles at time t = 1, on a 20 \times 18 polar grid

31/36

Kidder isentropic compression 0.8 0.7 0.7 0.6 0.5 0.2

Figure : Intial and final grids for a Kidder problem on a 10×5 polar mesh

(h) 2nd order

(g) 1st order

0.1

Kidder isentropic compression

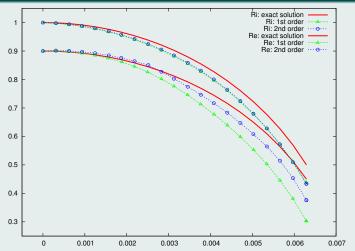


Figure: Interior and exterior shell radii evolution for a Kidder problem on a 10×5 polar mesh

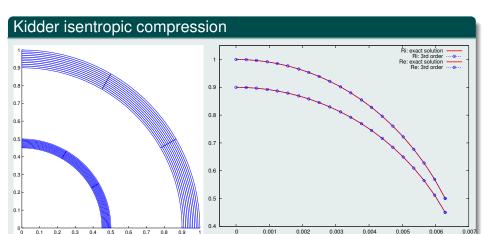


Figure : 3rd order solution for a Kidder compression problem on a 10 \times 3 polar grid

(j) Shell radii evolution

Initial and final grids

Accuracy and computational time for a Taylor-Green vortex

D.O.F	N	$E_{L_1}^h$	$E_{L_2}^h$	$E_{L_{\infty}}^{h}$	time (sec)
600	24 × 25	2.67E-2	3.31E-2	8.55E-2	2.01
2400	48 × 50	1.36E-2	1.69E-2	4.37E-2	11.0

Table: 1st order scheme

D.O.F	N	$E_{L_1}^h$	$E_{L_2}^h$	$E_{L_{\infty}}^{h}$	time (sec)
630	14 × 15	2.76E-3	3.33E-3	1.07E-2	2.77
2436	28 × 29	7.52E-4	9.02E-4	2.73E-3	11.3

Table: 2nd order scheme

D.O.F	Ν	$E_{L_1}^h$	$E_{L_2}^h$	$E_{L_{\infty}}^{h}$	time (sec)
600	10 × 10	2.67É-4	3.36Ē-4	1.21E-3	4.00
2400	20 × 20	3.43E-5	4.36E-5	1.66E-4	30.6

Table: 3rd order scheme

- - F. VILAR, P.-H. MAIRE AND R. ABGRALL, Cell-centered discontinuous Galerkin discretizations for two-dimensional scalar conservation laws on unstructured grids and for one-dimensional Lagrangian hydrodynamics. CAF, 2010.
- F. VILAR, Cell-centered discontinuous Galerkin discretization for two-dimensional Lagrangian hydrodynamics. CAF, 2012.
- F. VILAR, P.-H. MAIRE AND R. ABGRALL, A discontinuous Galerkin discretization for solving the two-dimensional gas dynamics equations written under total lagrangian formulation on general unstructured grids. JCP, 2014.
- F. VILAR, C.-W. SHU AND P.-H. MAIRE, Positivity-preserving cell-centered Lagrangian schemes for multi-material compressible flows: Form first-order to high-orders. Part I: The 1D case. JCP, 2016.
- F. VILAR, C.-W. SHU AND P.-H. MAIRE, Positivity-preserving cell-centered Lagrangian schemes for multi-material compressible flows: Form first-order to high-orders. Part II: The 2D case. JCP, 2016.

Taylor-Green vortex

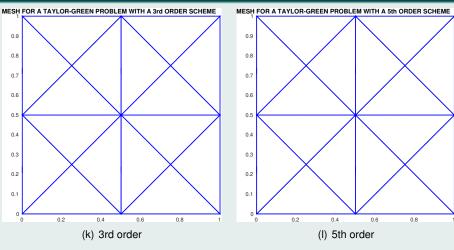


Figure : Final deformed grids at time t = 0.6, for 16 triangular cells meshes

Taylor-Green vortex

(k) 3rd order

(I) 5th order

Figure : Final deformed grids at time t = 0.6, for 16 triangular cells meshes

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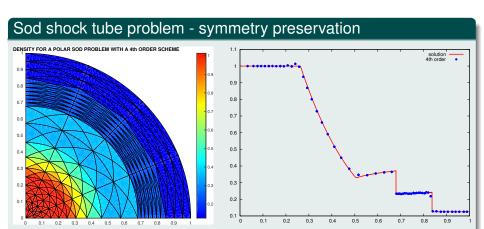


Figure: 4th order solution for a Sod shock tube problem on a polar grid made of 308 triangular cells

(n) Density profiles

(m) Density field

Sedov point blast problem - spurious deformations

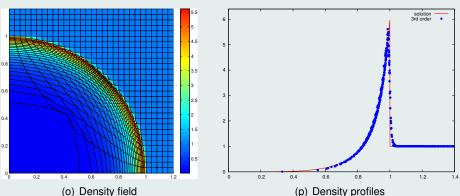


Figure : Third-order solution at time t=1 for a Sedov problem on a 30×30 Cartesian mesh