Institute of Theoretical and Mathematical Physics

Russian Federal Nuclear Center -

Anisotropic Closure Methods for Lagrangian Gas Dynamics and Elastoplasticity Equations in Mixed Cells

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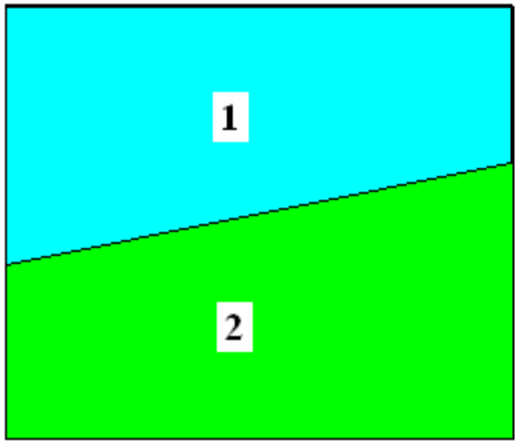
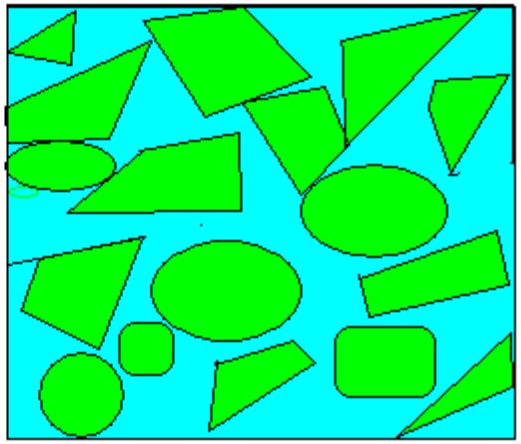
Introduction



interface



heterogeneous mixture

Mixed cells in ALE methods contain interfaces between different materials (left) or mixtures of materials (right).

Basic equations

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho}\nabla\cdot\mathbf{T}$$

$\mathbf{u}(u_x, u_y)$ is velocity (node-centered)
$\mathbf{T}$ is stress tensor

$$\frac{d\rho_\xi}{dt} = -\rho_\xi \nabla\cdot\mathbf{u}_\xi$$

ρ is density
ξ is material index

$$\frac{d\beta_\xi}{dt} = \beta_\xi\left(\nabla\cdot\mathbf{u}_\xi - \nabla\cdot\mathbf{u}\right)$$

β is volume fraction of the material ($\beta_\xi = V_\xi/V$)

$$\frac{de_\xi}{dt} = \frac{1}{\rho_\xi}\mathrm{Sp}(\mathbf{T}_\xi\mathbf{D}_\xi)$$

e is specific internal energy
$\mathbf{D}$ is strain rate tensor

$$\frac{d\mathbf{r}}{dt} = \mathbf{u}$$

$\mathbf{r}(x,y)$ – radius vector

$$T_{ij\xi} = S_{ij\xi} + \delta_{ij}P_\xi$$

$\mathbf{S}$ – stress tensor deviator

$$P_\xi = P_\xi\left(\rho_\xi, e_\xi\right)$$

equation of state

$$f_\xi = \left(\mathbf{S}_\xi, \mathbf{D}_\xi\right) = 0$$

model of matter

In the equations $P \to P+q$ and $P_\xi \to P_\xi + q_\xi$, q is artificial viscosity.

u_x, u_y are defined at node centers, ρ_ξ, β_ξ, e_ξ, P_ξ, $\mathbf{S}_\xi$ are defined in cells,

P, $\mathbf{S}$, q, q_ξ, $\mathbf{D}_\xi$, $\nabla\cdot u_\xi$ need to be defined.

Introduction of closure relations

$$p = \sum_\xi \psi_\xi p_\xi, \qquad q = \sum_\xi \psi_\xi q_\xi, \qquad \mathbf{S} = \sum_\xi \psi_\xi \mathbf{S}_\xi \tag{1}$$

where ψ_ξ is defined by the closure model adopted.

$\nabla \cdot u_\xi$, ψ_ξ, q_ξ, $\mathbf{D}_\xi$ are not defined. Closure relations are needed.

Their introduction is subject to conservation laws.

Requirement 1 is additivity of volumes ("volume" conservation)

$$V = \sum_\xi V_\xi, \quad \text{or} \quad \sum \beta_\xi = 1 \longrightarrow \Delta V = \sum_\xi \Delta V_\xi, \quad \text{or} \quad \sum \beta_\xi \nabla \cdot \mathbf{u}_\xi = \nabla \cdot \mathbf{u} \tag{2}$$

Natural extension of (2) is

$$\sum_\xi \beta_\xi \mathbf{D}_\xi = \mathbf{D} \quad \text{satisfied at} \quad \mathbf{D}_\xi = \mathbf{D} \cdot \left(\frac{\nabla \cdot \mathbf{u}_\xi}{\nabla \cdot \mathbf{u}} \right) \tag{3}$$

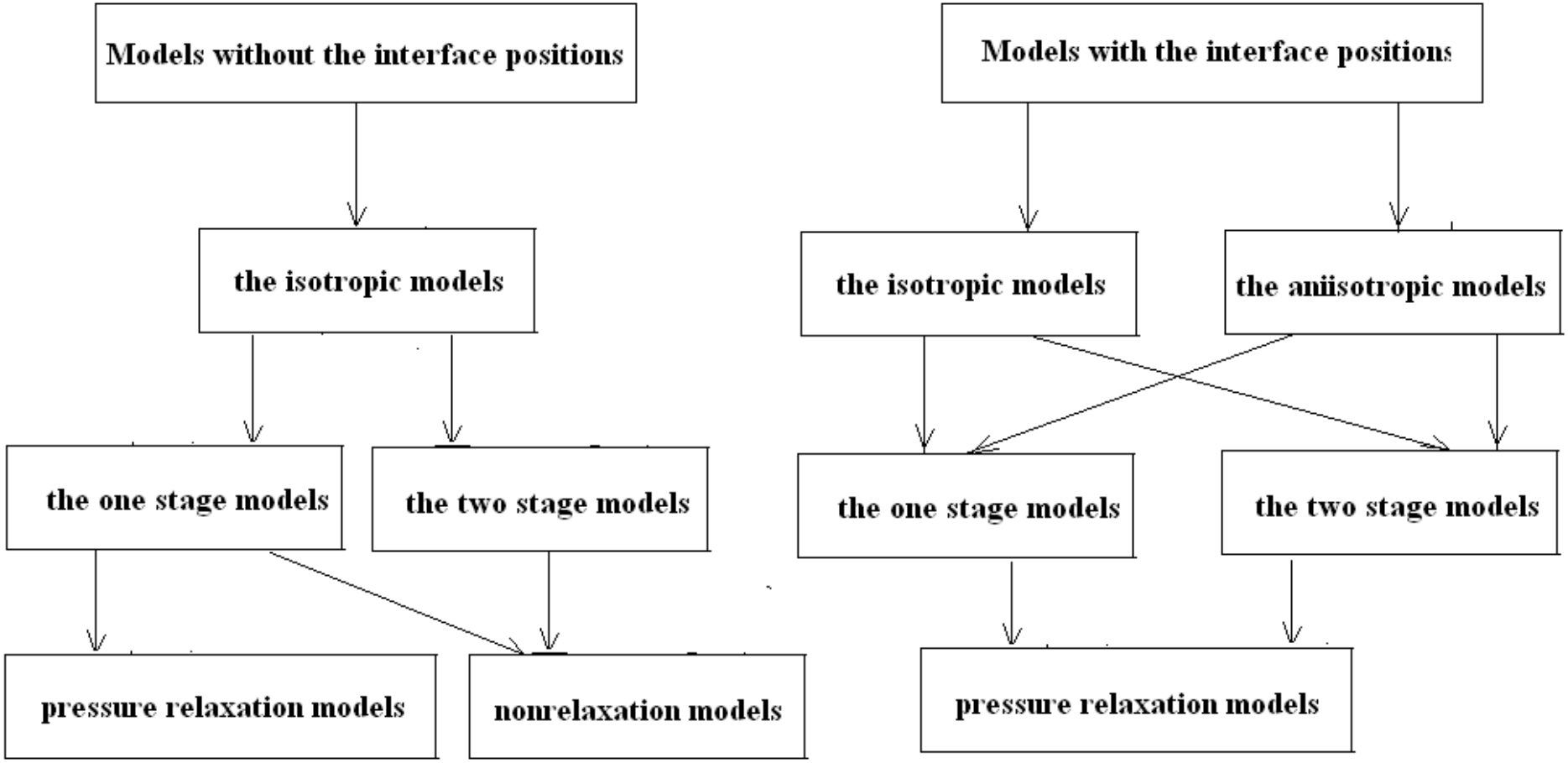
Requirement 2 is additivity of energies (energy conservation)

$$e = \sum \alpha_\xi e_\xi \longrightarrow \Delta e = \sum \alpha_\xi \Delta e_\xi \qquad \text{where} \quad \alpha_\xi = M_\xi / M \tag{4}$$

Thus, the basic parameter to be defined by the closure model is $\nabla \cdot u_\xi$

The second parameter is q_ξ

Classification of the models



Isotropic single-stage closure methods

Relaxation methods

Two methods based on the model of equal pressures of materials.

$$p_\xi = p, \tag{5}$$

1. Harlow's method [Harlow, 1964];
2. Tipton's method [Tipton, 1989];

3. Delov's method based on the acoustic Riemann solver (Delov) [Delov, Sadchikov, 2005] (this model also underlies the DSS [Kamm, Shashkov, Fung, Harrison, Canfield, 2010] and the KSR [Kamm, Shashkov, Rider, 2011]) methods developed later;

4. K&S method based on the Riemann solver [Kamm, Shashkov, 2010].

Isotropic single-stage closure methods

Non-relaxation methods

5. The methods based on the equal compressibilities of materials ($\nabla \cdot \mathbf{u}$) [Бахрах, Спиридонов, Шанин, 1984; Benson, 1992];

$$\nabla \cdot \mathbf{u}_\xi = \nabla \cdot \mathbf{u}_\zeta = \nabla \cdot \mathbf{u} \qquad (7)$$

6. The methods based on the equal pressure increments of materials (Δp) [Bondarenko, Yanilkin, 2002];

$$\Delta p_\xi = \Delta p_\zeta \qquad (8)$$

7. The methods based on equal velocities of materials behind weak shock (Δu) [Goncharov, Kolobyanin, Yanilkin, 2006];

$$u_\xi = u_\zeta \qquad (9)$$

Isotropic two-stage closure methods

Two-stage models include the stage of subscale interactions between the materials in the non-equilibrium state; so the first stage here can only use models 5-7. This approach for closure models has been proposed independently in [Barlow, 2001] and [Goncharov, Yanilkin, 2004].

The subscale pressure relaxation method (**the PR method**) from [Goncharov, Yanilkin, 2004] is versatile and it is used jointly with models 5-7 denoted below as the $\nabla\cdot\mathbf{u}$-PR, Δp-PR and Δu-PR methods (Pressure Relaxation).

All the above methods do not employ the interface location inside a mixed cell. However, there are methods that make essential use of this information. A method of this kind was first proposed in [Barlow] and then developed in the "interface-aware sub-scale dynamics" IA-SSD method [Hill, Barlow, Shashkov, 2014] for the multi-material cell case. It is a two-stage method, the first stage in which employs the $\nabla\cdot\mathbf{u}$ model. The second (subscale) stage uses the model based on the acoustic Riemann solver (**Delov's** model).

Pressure relaxation method (method PR)

Materials' pressure relaxation is done in the adiabatic approximation subject to the requirement that total divergence and energy remain constant at this stage. The formula for the materials' divergence is

$$\nabla \cdot \mathbf{u}_\xi = -\frac{\Delta p_\xi}{\tau \rho_\xi c_\xi^2} \qquad \Delta p_\xi = A\, c\tau / h \left(p - p_\xi \right) \qquad A \sim 1, \qquad (10)$$

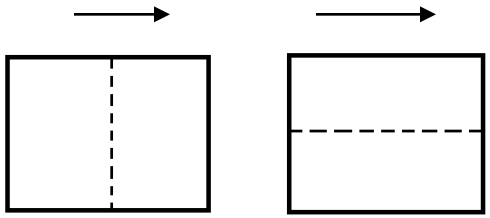
where p is common pressure $p = \sum \beta_\xi p_\xi$

ΔE

Anisotropic closure methods

1 Concept

Let us consider two limiting cases of interface location relative to the wave motion (shock, acoustic or elastic wave)



In the first case (left figure), velocity is mostly normal to the interface, so all the above models are suitable.

In the second case (right), velocity is mostly directed along the interface, while lateral velocity is insignificant. It means that the materials contract or expand tangentially to the interface; thus, equality of divergences may be more consistent in this case.

Thus, to ensure acceptable modeling accuracy for the two different types of flow, different closure relations need to be used.

For this purpose, two-stage models are proposed.

Like above, we represent the total divergence as a sum of two items

$$\nabla \cdot \mathbf{u}_{\xi} = \nabla \cdot \mathbf{u}_{\xi 1} + \nabla \cdot \mathbf{u}_{\xi 2}$$

The two methods differ in the ways of their determination.

ΔE

Anisotropic closure methods

1 Method ACM-1

The **first** stage uses the model of equal divergences giving

$$\nabla \cdot \mathbf{u}_{\xi 1} = \nabla \cdot \mathbf{u}$$

At the **second** stage, the pressures of the mixed cell materials get relaxed according to an algorithm, which is basically the same as the PR algorithm.

$$\nabla \cdot \mathbf{u}_{\xi 2} = -\frac{\Delta p_\xi}{\tau \rho_\xi c_\xi^2} \qquad \Delta p_\xi = A\, c\tau/h\left(p - p_\xi\right) \qquad A\ (\text{constant}) \sim 1,$$

The only distinguishing feature is that for the ACM-1 model, the factor A depends on the mutual orientation of velocity and interface directions.

The total divergence is written as the sum of two components:

$$\nabla \cdot \mathbf{u} = \nabla \cdot \mathbf{u}_\tau + \nabla \cdot \mathbf{u}_n$$

Suppose $A = A_0 \cdot \dfrac{\nabla \cdot \mathbf{u}_n}{\nabla \cdot \mathbf{u}}$ A_0 is some constant $(A_0 = 1)$

Thus, the factor A is variable in this case.

If the velocity is normal to the interface $\nabla \cdot \mathbf{u}_n = \nabla \cdot \mathbf{u}$, $A = A_0$

If the velocity is directed along the interface $\nabla \cdot \mathbf{u}_n = 0$, $A = 0$

ΔE

Anisotropic closure methods

2 Method ACM-2

We decompose the divergence of the entire cell and its materials into two components: normal and tangential (relative to the interface location):

$$\nabla\cdot\mathbf{u}=\nabla\cdot\mathbf{u}_{\tau}+\nabla\cdot\mathbf{u}_{n}\qquad \nabla\cdot\mathbf{u}_{\xi}=\nabla\cdot\mathbf{u}_{\xi\tau}+\nabla\cdot\mathbf{u}_{\xi n}$$

The materials are assumed to have equal compressibilities along the interface

$$\nabla\cdot\mathbf{u}_{\xi\tau}=\nabla\cdot\mathbf{u}_{\tau}$$

For divergence in the direction normal to the interface, one can use any of the closure models (1, 5-7); we use the model $\Delta u_{\xi}=\Delta u_{\zeta}$

$$\nabla\cdot\mathbf{u}_{\xi n}=\lambda_{\xi}\nabla\cdot\mathbf{u}_{n}$$

$$\lambda_{\xi}=\frac{1}{c_{\xi}}\sum_{k}\frac{\beta_{k}}{c_{k}}$$

Once this part of the divergence is distributed to the materials, relaxation of their pressures is done by the PR method, which makes an additional contribution, $\nabla\cdot\mathbf{u}'_{\xi n}$, to the divergence $\nabla\cdot\mathbf{u}_{\xi n}$

$$\widetilde{\nabla\cdot\mathbf{u}}_{\xi n}=\nabla\cdot\mathbf{u}_{\xi n}+\nabla\cdot\mathbf{u}'_{\xi n}$$

Ultimately, $$\nabla\cdot\mathbf{u}_{\xi}=\widetilde{\nabla\cdot\mathbf{u}}_{\xi n}+\nabla\cdot\mathbf{u}_{\xi\tau}$$

ΔE

Method for calculating mixed cells with vacuum

One of the materials available in EGAK is a zero-pressure “vacuum”. For the case of vacuum, a special algorithm has been developed, which is the same for closure methods 1, 5-7. The development of this algorithm was motivated by the fact that the pressure for vacuum is specified rather than controlled by the closure method.

In a mixed cell with vacuum, two cases are possible: $\nabla \cdot \mathbf{u} > 0$ и $\nabla \cdot \mathbf{u} \le 0$

Case $\nabla \cdot \mathbf{u} > 0$ **;** it is assumed that $\nabla \cdot \mathbf{u}_\xi = \nabla \cdot \mathbf{u}$

Case $\nabla \cdot \mathbf{u} \le 0$ **;** cell volume is assumed to decrease only through a decrease in vacuum volume.

For the ACM-1 and ACM-2 methods, the total divergence is represented as a sum:

$$\nabla \cdot \mathbf{u} = \nabla \cdot \mathbf{u}_\tau + \nabla \cdot \mathbf{u}_n$$

If the cell expands, $\nabla \cdot \mathbf{u} \ge 0$ $\nabla \cdot \mathbf{u}_\xi = \nabla \cdot \mathbf{u}$

At $\nabla \cdot \mathbf{u} < 0$, two cases are possible:

- if $\nabla \cdot \mathbf{u}_n < 0$ then $\nabla \cdot \mathbf{u}_\xi = \nabla \cdot \mathbf{u}_{\xi\tau}$ $\nabla \cdot \mathbf{u}_{vac} = \nabla \cdot \mathbf{u} - \dfrac{\beta_\xi}{\beta_{vac}} \cdot \nabla \cdot \mathbf{u}_\xi$
- if $\nabla \cdot \mathbf{u}_n \ge 0$ then $\nabla \cdot \mathbf{u}_\xi = \nabla \cdot \mathbf{u}$

ΔE

Artificial viscosity

In addition to the methods discussed above, mixed cells require relations to calculate artificial viscosity for the materials. Six approaches are considered in [Goncharov, Kolobyanin, Yanilkin, 2010]. The best of them is number 3.

1	equal to the cell-average viscosity	$q_\xi = q$
2	viscosity with its quantities $\rho_\xi, h_\xi = \beta_\xi h, \nabla \cdot \mathbf{u}_\xi$	$q_\xi = q \dfrac{\rho_\xi \beta_\xi^2 \lambda_\xi^2}{\sum \rho_k \beta_k^3 \lambda_k^3}$
3	proportional to material densities $q_\xi \sim \rho_\xi$	$q_\xi = q \dfrac{\rho_\xi}{\sum \rho_k \beta_k \lambda_k}$
4	equal pressure increments $\Delta p_\xi = \Delta p_\zeta$	$q_\xi = q \dfrac{\rho_\xi}{\lambda_\xi \left(\dfrac{\partial p_\xi}{\partial e_\xi}\right)_\rho \sum \dfrac{\beta_k \rho_k}{(\partial p_k / \partial e_k)_\rho}}$
5	equal energy increments $\Delta e_\xi = \Delta e_\zeta$	$q_\xi = q \dfrac{\rho_\xi}{\rho \lambda_\xi}$
6	proportional to pressure increment $q_\xi \sim \Delta p_\xi$	$A \cdot \rho_\xi c_\xi^2 = \left(\partial p_\xi / \partial e_\xi\right)_\rho q_\xi / \rho_\xi$ A is proportionality factor

ΔE

Test problems and results

The following unified types of data processing are presented for the 1D problem simulations.

1. Plots of convergence in the L_1 norm.

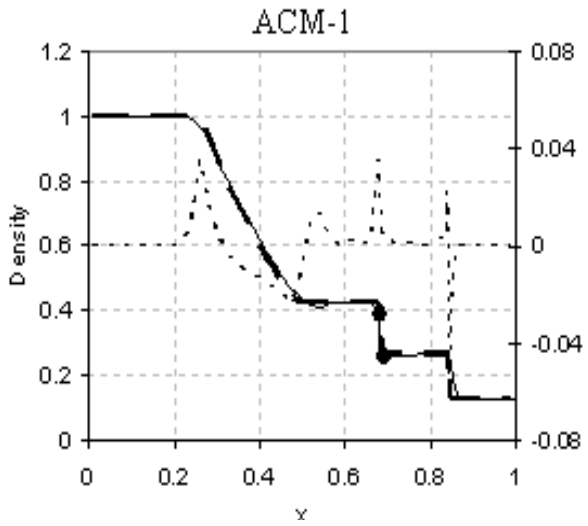
2. Tabulated quantities characterizing the order of convergence of integral error of basic quantities in the L_1 norm.
   The error is calculated by the formula

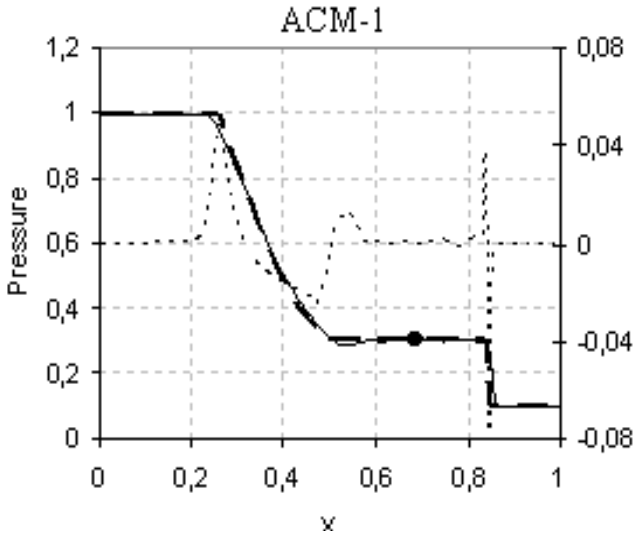
$$\delta y = \left\| y_{comp} - y_{exact} \right\|_1 = Ah^{\sigma}$$

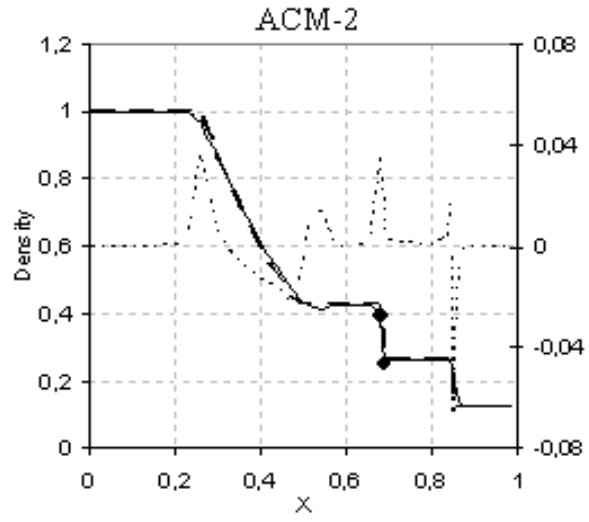
where h is the initial mesh spacing, y_{comp}, y_{exact} are the calculated and the exact value of the quantity at the cell center.

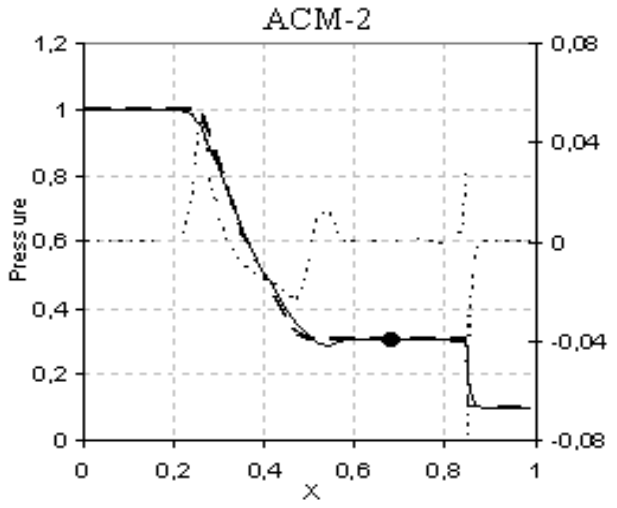
3. Tabulated values of basic quantities in mixed cells.

1. Sod problem



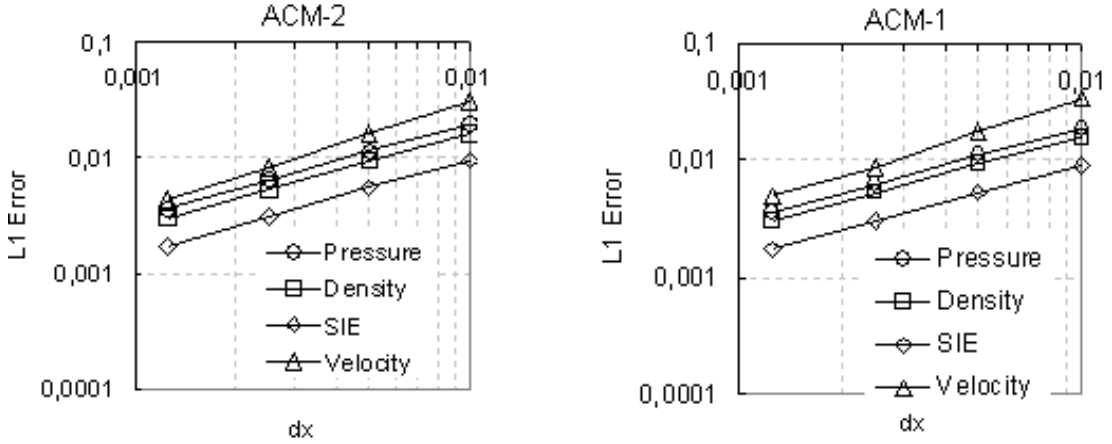






Sod problem

Plots of convergence in the L_1 norm



Convergence parameters

L_1	100	200	400	800	A	σ
p	1.89E-02	1.11E-02	6.33E-03	3.58E-03	1.89E-02	0.80
ρ	1.58E-02	9.39E-03	5.35E-03	3.01E-03	1.59E-02	0.80
e	9.09E-03	5.42E-03	3.01E-03	1.71E-03	9.22E-03	0.81
u	3.40E-02	1.78E-02	8.66E-03	4.99E-03	3.45E-02	0.93

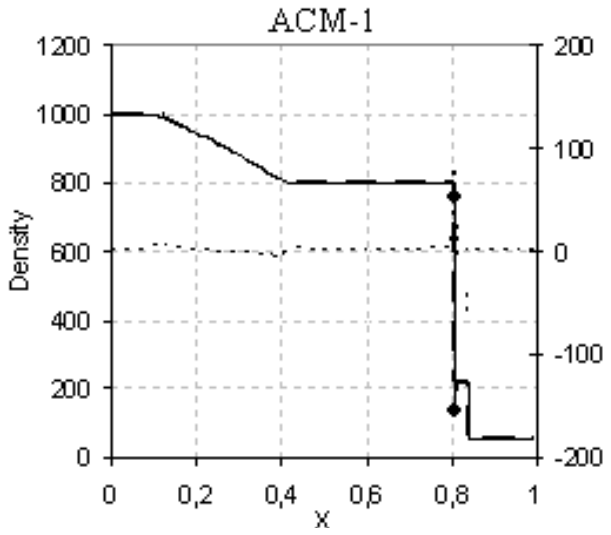
ACM-2

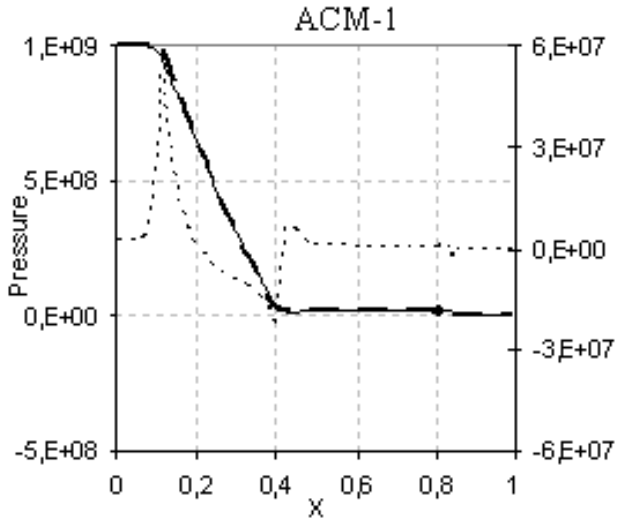
L_1	100	200	400	800	A	σ
p	1.96E-02	1.13E-02	6.44E-03	3.60E-03	1.97E-02	0.81
ρ	1.63E-02	9.51E-03	5.40E-03	3.01E-03	1.65E-02	0.81
e	9.53E-03	5.51E-03	3.08E-03	1.71E-03	9.64E-03	0.83
u	3.11E-02	1.61E-02	8.30E-03	4.29E-03	3.11E-02	0.95

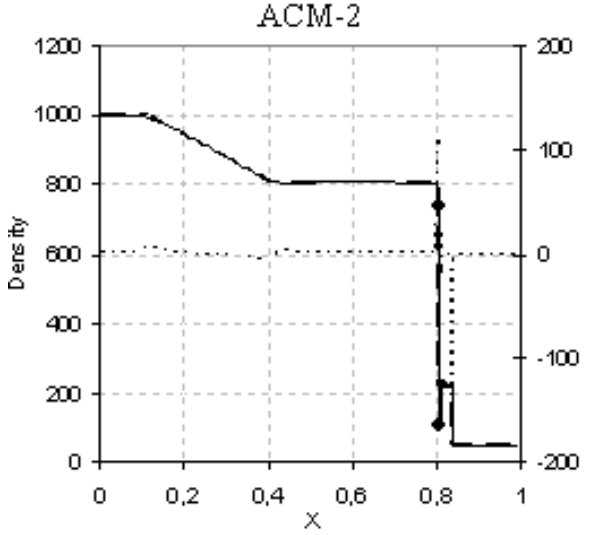
ACM-1

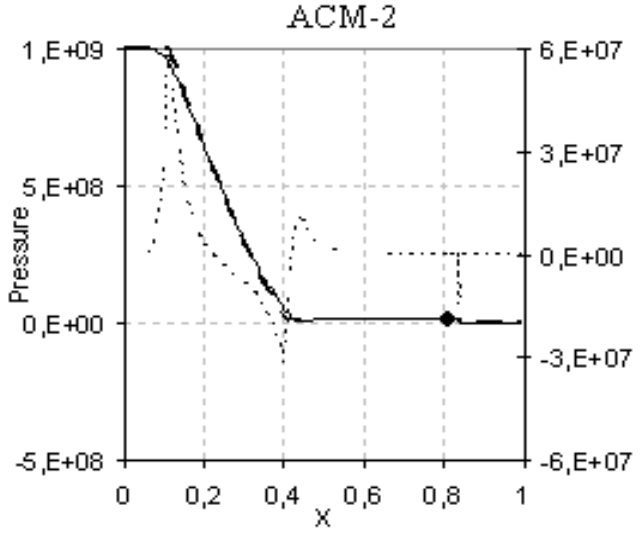
2. Water-air shock tube problem

(Plohr, 1988; Saurel, Abgrfll, 1999)



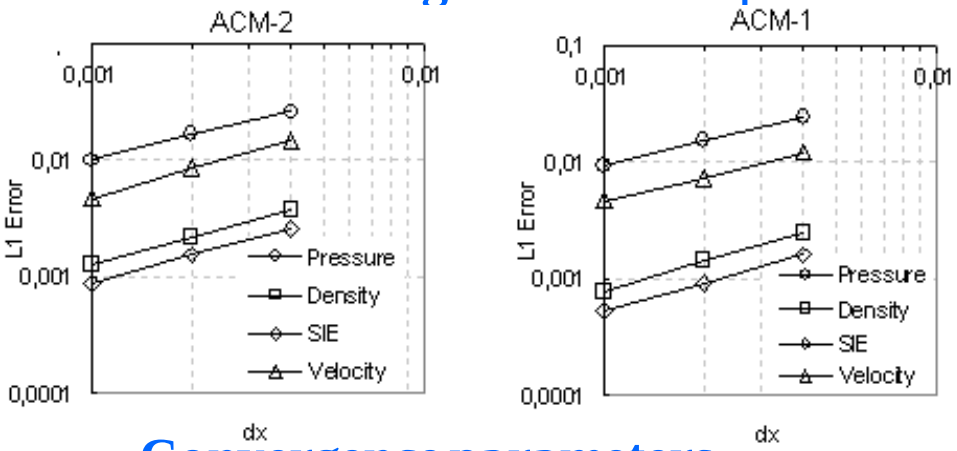






Water-air shock tube problem

Plots of convergence in the L_1 norm



Convergence parameters

L_1	250	500	1000	A	σ
p	2.39E-02	1.53E-02	9.37E-03	2.39E-02	0.68
ρ	2.51E-03	1.44E-03	7.93E-04	2.51E-03	0.83
e	1.64E-03	9.19E-04	5.29E-04	1.64E-03	0.81
u	1.22E-02	7.13E-03	4.69E-03	1.22E-02	0.69

ACM-2

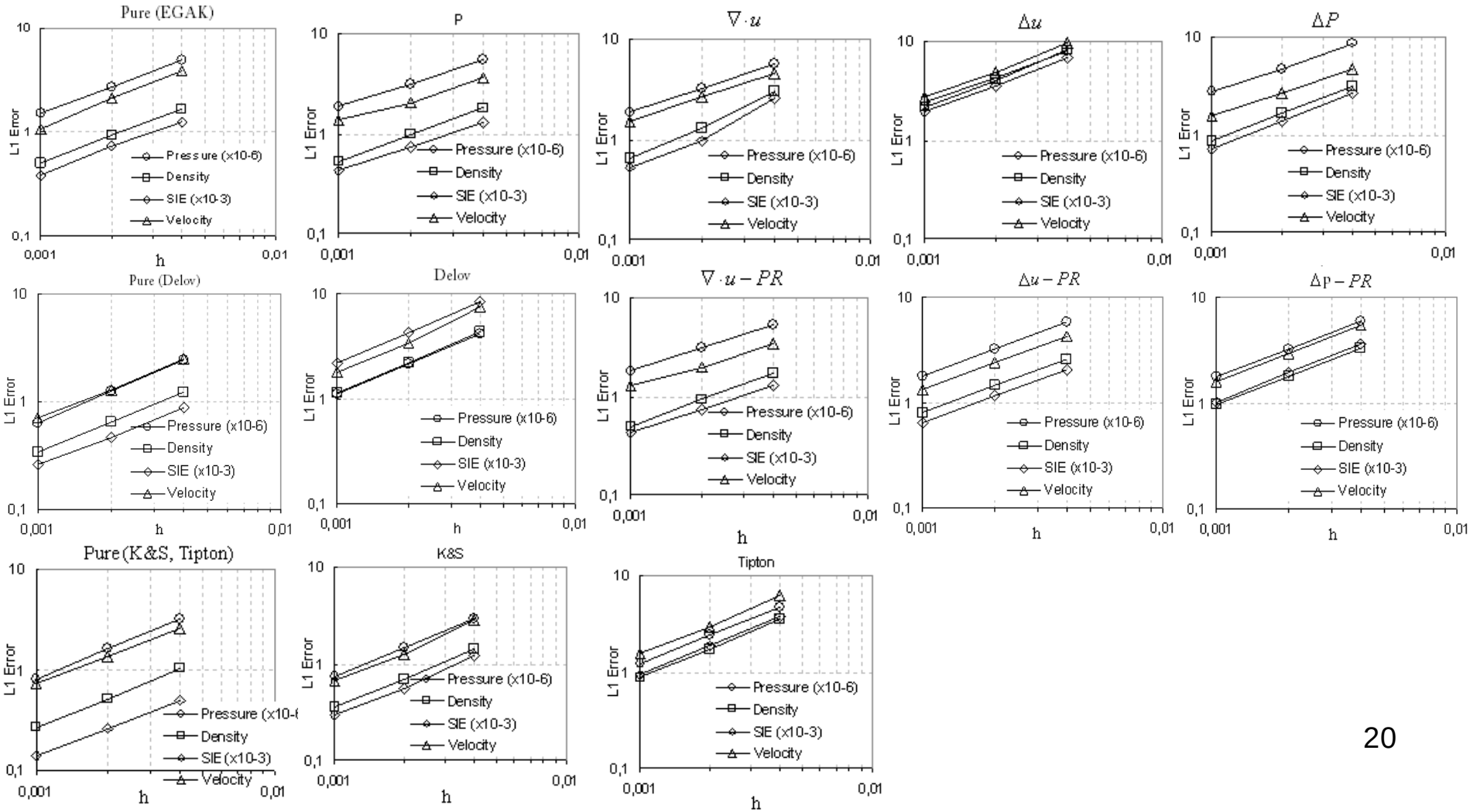
L_1	250	500	1000	A	σ
p	2.55E-02	1.66E-02	1.00E-02	2.58E-02	0.68
ρ	3.73E-03	2.23E-03	1.28E-03	3.76E-03	0.77
e	2.63E-03	1.57E-03	8.93E-04	2.65E-03	0.78
u	1.51E-02	8.52E-03	4.76E-03	1.51E-02	0.83

ACM-1

2. Water-air shock tube problem

(Plohr, 1988; Saurel, Abgrfll, 1999)

Plots of convergence in the L1 norm



3. Mixed-material shock transition problem

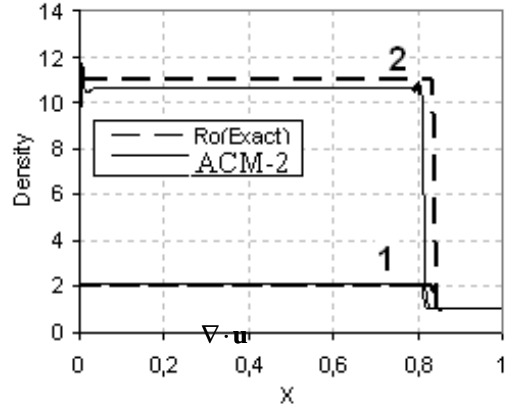
Initial data $$(\gamma, \rho, e, p, u, \beta) = \begin{cases} (3.0,\ 1.0,\ 0.,\ 0.,\ 0,\ 0.5\ ), & \text{if } -2.0 \le x \le 1.0, \\ (1.2,\ 1.0,\ 0.,\ 0.,\ 0),\ 0.5) & \text{if } -2.0 \le x \le 1.0 \end{cases}$$

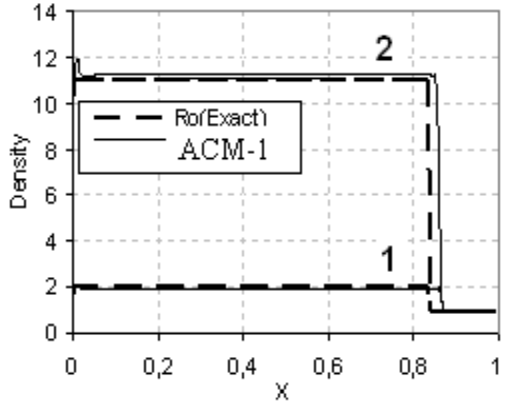
Velocity at the boundary is constant u_x=2, EoS is ideal gas.

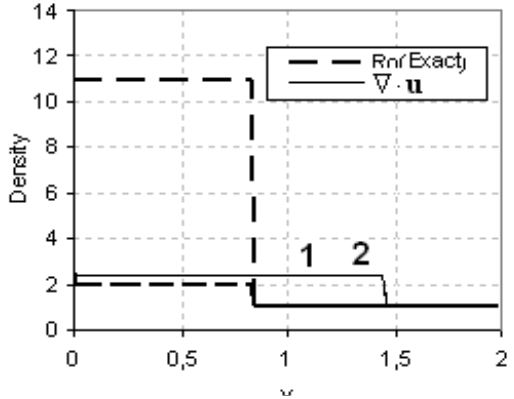
The problem has an analytical solution obtained by Goncharov assuming that the materials have equal pressures.

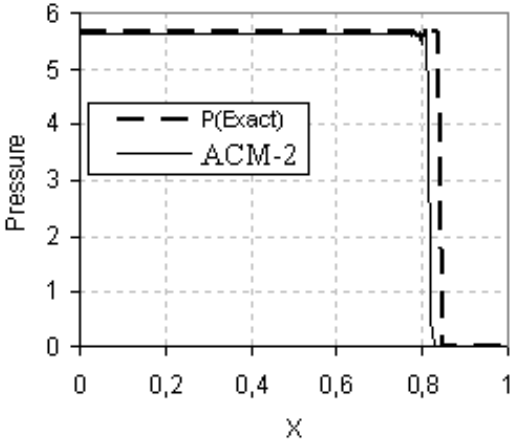
This problem differs from the two above. First, there are no pure cells, so pure-cell simulations are inapplicable. Second, only some of the above plots can be obtained for it. In particular, it makes almost no sense to perform convergence calculations for this problem, because the steady-state solution in the mixed cells does not depend on the mesh spacing.

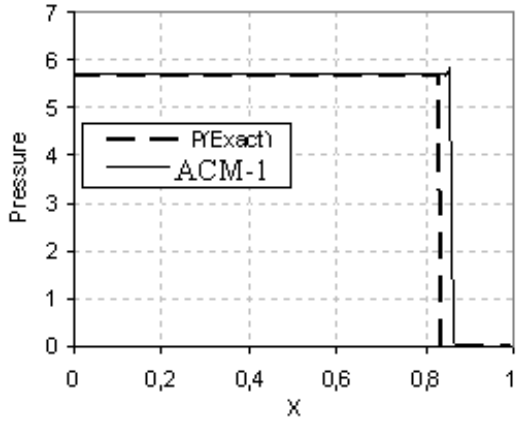
3. Mixed-material shock transition problem

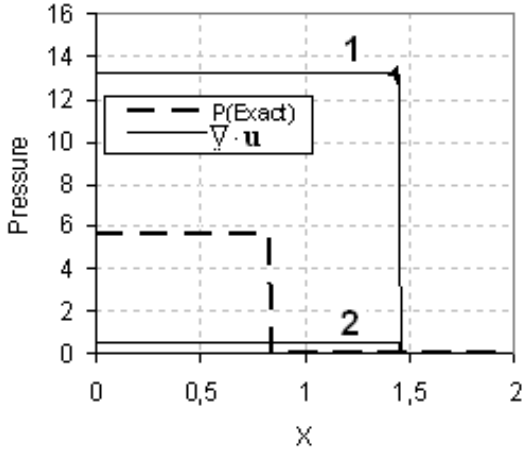












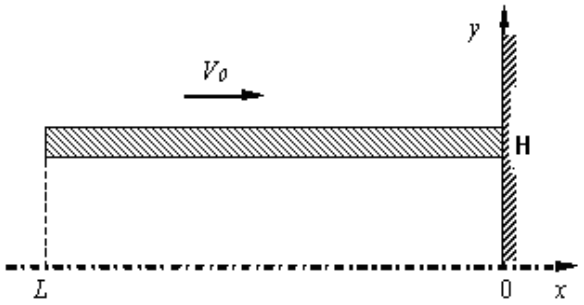
3. Mixed-material shock transition problem

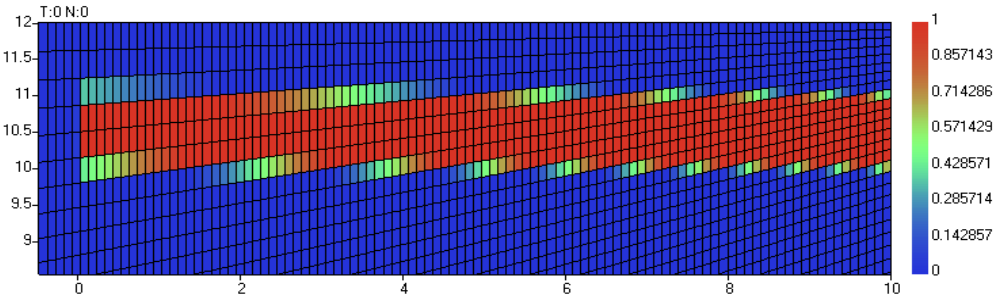
Steady-state quantities in a mixed cell

метод	D	p_1	p_2	ρ_1	ρ_2	e_1	e_2
exact	2.839	5.677	5.677	2.0	11	1.419	2.581
$\nabla \cdot \mathbf{u}$	3.456	13.219	0.581	2.379	2.379	2.778	1.222
Δu	2.827	5.886	5.324	2.053	10.372	1.434	2.567
$\nabla \cdot \mathbf{u}$ -PR (ACM-1)	2.859	5.715	5.715	1.956	11.253	1.461	2.539
Δu-PR (ACM-2)	2.817	5.640	5.640	2.047	10.754	1.378	2.622

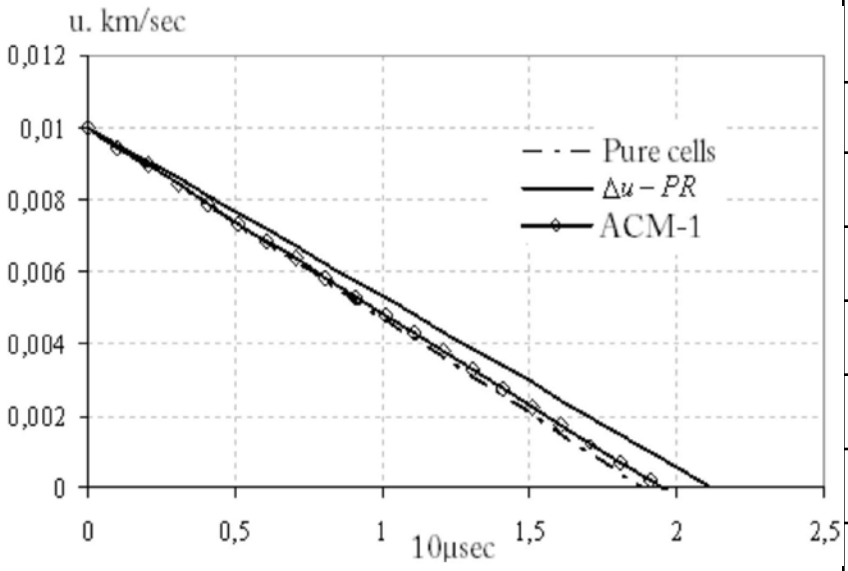
4. 2D problem of elastic wave in a plate

(proposed by A. Krayukhin)





The plate is titanium surrounded with vacuum or air; it is flying at v_0=0.01 km/s and hitting a rigid wall; as a result, an elastic wave is propagating in the plate.



closure method	surrounding medium	c_w, km/s
exact		**5.3**
pure cells	air	5.3
Δu-PR	vacuum	4.8
ACM-1	vacuum	5.1
ACM-2	vacuum	5.1
ACM-1 (oblique mesh)	vacuum	5.1
Δu-PR	air	4.7
ACM-1	air	5.1

Discussion of results and conclusions

The simulations – both presented here and not included in this overview – demonstrate that all the methods under consideration have good convergence (~1) to the exact solution with decrease in the mesh spacing on all the 1D problems. Note that the order of convergence of the simulations with closure methods is basically controlled by that of the main difference scheme. As for the error of the closure methods themselves, it is basically controlled by the value of the factor A in the error formula

$$\delta y = \left\| y_{comp} - y_{exact} \right\|_1 = Ah^{\sigma}$$

You can choose the method you like. However, two circumstances need to be mentioned, which are important when choosing the method. First, the methods differ in the amount of calculations. Second, the methods differ in the complications in program implementation associated with limitations in their applicability.

As for the 2D problem, the anisotropic methods have no alternative. They possess the same accuracy as the basic methods on the 1D problems, because they rest upon the same closure models, and are more accurate as applied to the 2D problem. Of the two anisotropic methods, preference can be given to ACM-1, because it is easier to implement.

Thank you for attention

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