Cluster Dynamics Method for Simulation of Dynamic Processes of Continuum Mechanics

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- Introduction
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Introduction

- Cluster dynamics method (CDM) developed in VNIIEF is one of the variants of particle method intended for simulation of the processes associated with large deformations and continuity violation of the material.
- In numerical simulation it is based on molecular dynamics method, but the basic advantage of CDM is the possibility to choose the base cluster, that allows the simulation of the processes in a wide range of spatial scales (from micrometer to tens of centimeters).

Introduction

- By now we have performed the construction procedure for cluster interaction potentials corresponding to real equations of state of material by the example of typical metals. Numerical simulation of shock wave arrival at profiled plate surface, high-velocity target penetration and production problems were carried out using CDM. The computational results are compared with experimental data and other computational results.
- The results show that CDM can be used for full-scale simulation of large deformation and dynamic fracture of materials at impulse loading at characteristic rates of relative deformation of 10^3-10^6 s^{-1}.

Cluster dynamics method

The following assumptions serve as the basis of the cluster dynamics method:

- continuum representation as a set of distinguished units (point base cluster);
- substitution of continuum mechanics equations for equations of motion of interacting clusters;
- application of molecular dynamics method to describe the dynamics of cluster motion;
- selection of cluster interaction potential based on the real equation of state of the simulated material.

As the given method assumes the discrete structure of the medium, there are no essential difficulties in describing the fracture, continuity violation, structure change and others.

Cluster Dynamics Method

For simplicity accept the classical equations of cluster motion, the interactions are considered to be pair, and the force is considered to act in radius-vector direction between the particles:

$$m\ddot{\vec{r}}_k = \sum_{n=1}^{N} \vec{f}\left(\left|\vec{r}_k - \vec{r}_n\right|, \theta, \varphi\right) \qquad (1)$$

where – radius vector of *k* particle,
m – particle mass, *N* – the total quantity of particles,

$\vec{f}(r,\theta,\varphi) = -\nabla V(\vec{r})$ – interaction force between the particles

corresponding to the interaction potential V(r).

Cluster dynamics method

- Base cluster quantities (mass, equilibrium distance between the particles) are chosen to reproduce the peculiarities of the initial geometry and real size of the problem, and on the other hand to provide the computations for the true time (true working hours).
- The freedom in choosing the cluster dimension (conserving medium density and region size) means that the initial equations should be of certain scale invariance. Thus, for the sake of self-consistency of the approach, the interaction potential transformation law should be defined at changing base cluster parameters.

Cluster dynamics method

Postulate the following transformation law
of pair particle interaction *U* changing base cluster dimension:

$$V(r,a,m)=\frac{m}{m_0}V_0\left(r\frac{a_0}{a}\right) \qquad (2)$$

Form physical point of view (2) means that force stress
is defined by relative deformation, and dynamics of the processes
should not be dependent on simulation cluster quantities.
The form (2) provides the independence of basic mechanical
characteristics of the medium on cluster dimensions,
it also gives one and the same field
of directed velocities of the particles in calculations.

Cluster dynamics method

- Note that the clusters introduced above should not be associated with physical particles; they are mathematical simulation objects used for the further averaging and serve as medium marker similarly to SPH method.
- However, it is important that cluster dimension does not influence the obtained macroscopic flow pattern as well as the distribution of averaged quantities (energy, pressure, velocity, density) which allows the use of CDM for numerical simulation of continuum mechanics dynamic processes.

Cluster interaction potentials

- It is very important to choose the functional dependence for *U(r)* potential for CDM implementation. We find this dependence using equations of state of the materials.

Mie-Grüneisen equation of state

$$\varepsilon_x(\delta) = \frac{c_0^{\,2}}{n}\left(\frac{\delta^{n-1}-1}{n-1}+\frac{1}{\delta}-1\right)$$

where $\delta=\rho/\rho_0$, и c_0,
n – variables of the equation of state

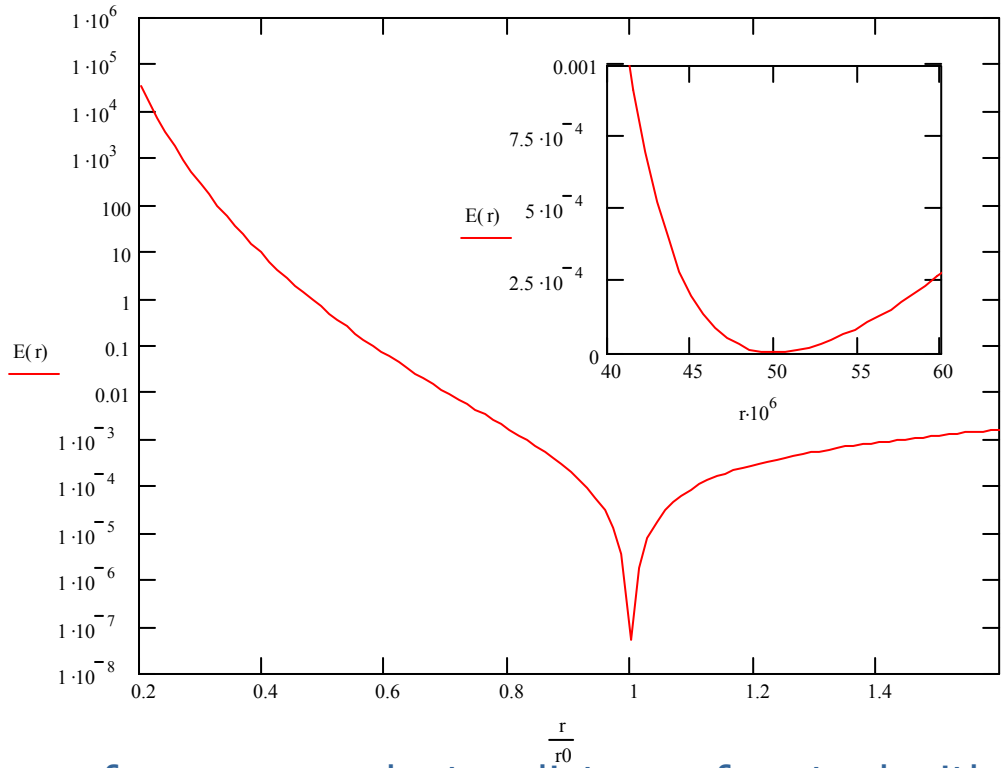
$$E\ (r) = \frac{\sqrt{2}\rho_0 r_0^3 c_0^2}{12n}\left[\frac{\left(\frac{r_0}{r}\right)^{3n-3}-1}{n-1}+\left(\frac{r}{r_0}\right)^3-1\right]$$

$$m_0 = \frac{\rho_0 r_0^3}{\sqrt{2}}$$

For space initial closest-packed clusters

- Cluster interaction potentials found like that will allow for the behavior of dynamic compression and external loading extension of the metals.

Cluster interaction potentials

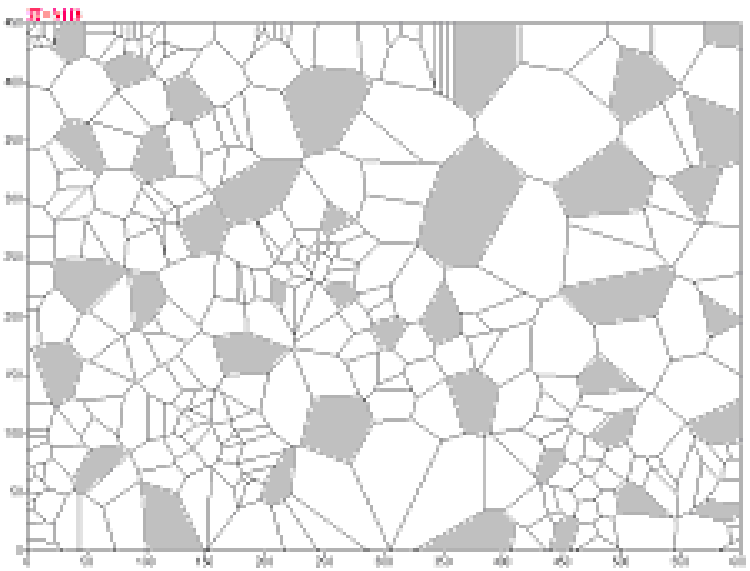


Dependence of energy on cluster distance for steel with Mie-Grüneisen equation of state parameters:

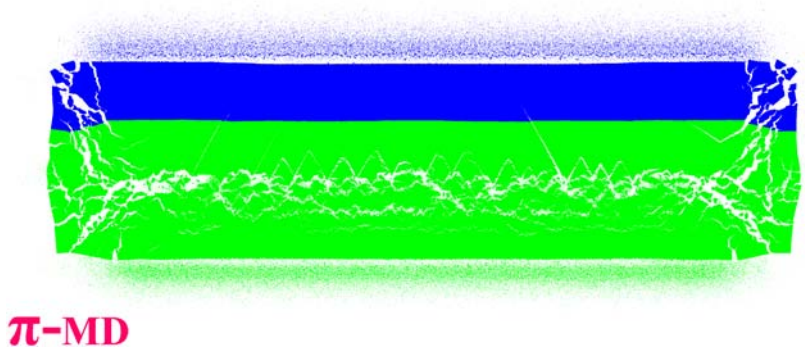
ρ_0=7.8 g/cm³, c_0=4.9 km/s, n=5, r_0=50 mkm.

Cluster interaction potentials

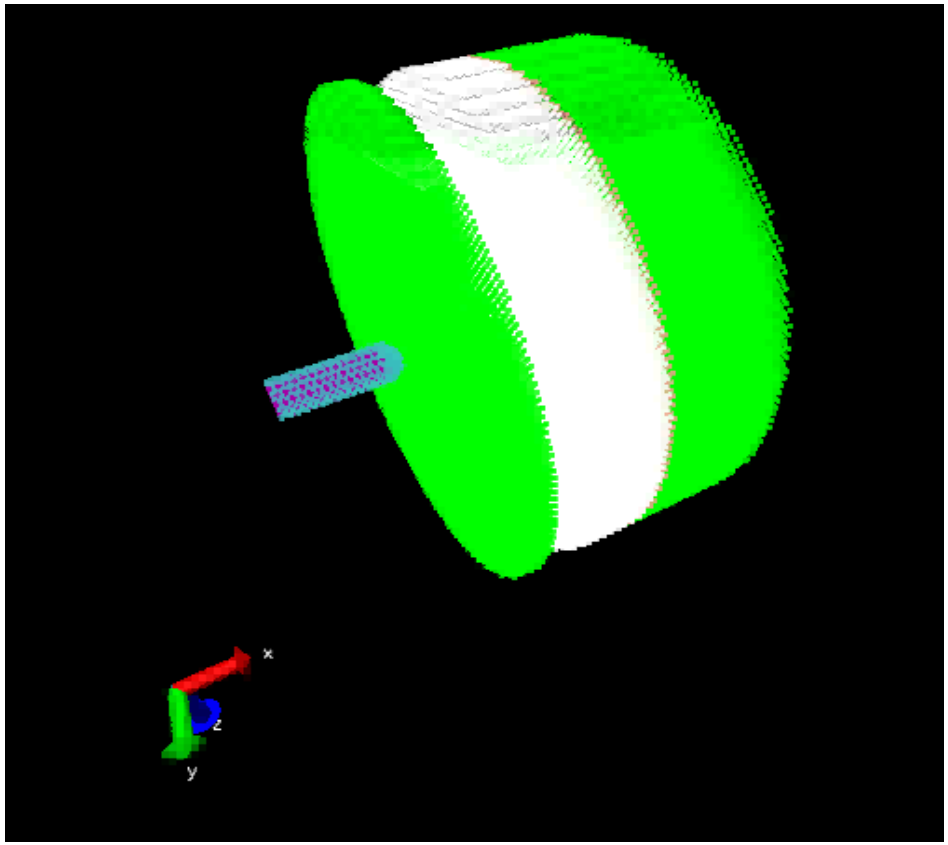
Heterogeneous material model



Different material plate collision



Cluster interaction potentials



Penetration of multilayer shield

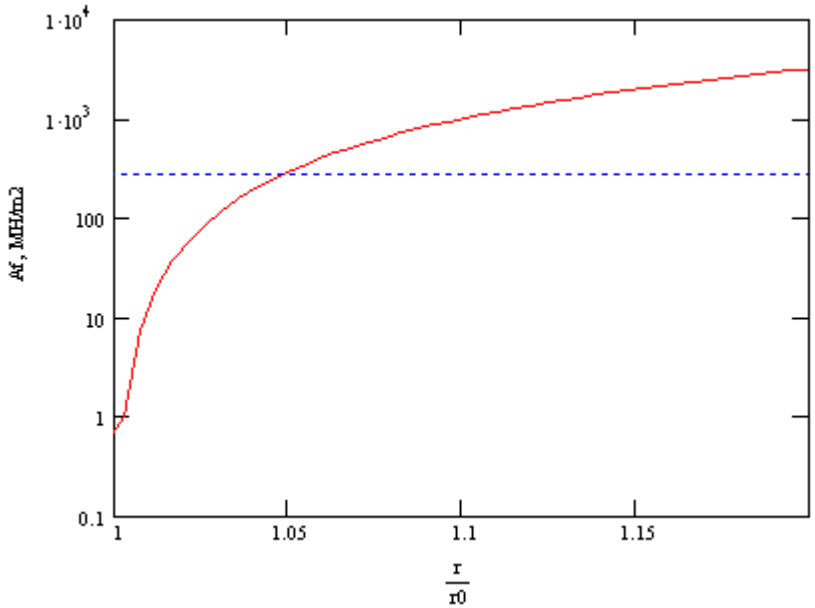
Cluster interaction potentials

Specific fracture energy of different metals*

Material	A_f, MH / m²
Brass	233
Stainless steel	275
Aliminium	95

*Physics of explosion/edited by L.P. Orlenko. V2,-M. FIZMATLIT,2002

Computational dependence of specific fracture energy on potential cut-off radius



Steel: ρ_0=7.8 g/cm³, c_0=4.9 km/s, n=5, r_0=50 μm.

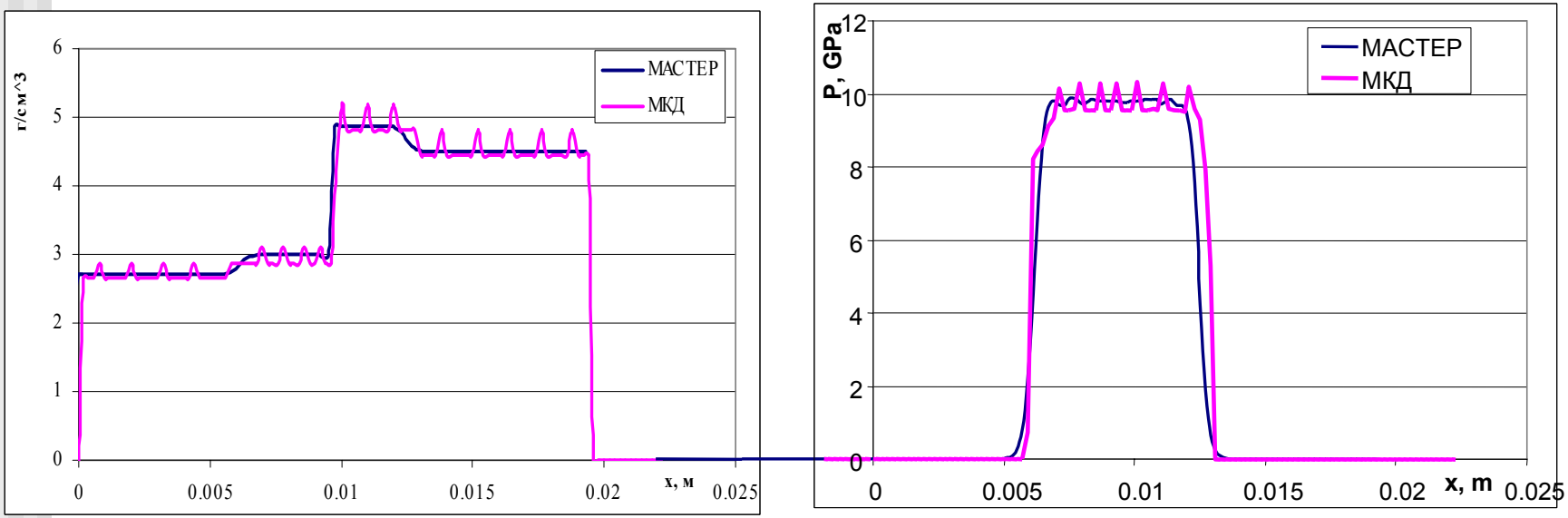
CDM application

CDM method has been verified using the following problems with experimental data provided:

- collision of aluminum and titanium plates moving at relative velocities 1 km/s;
- aluminum projectile penetration of thick aluminum plate at initial velocity ~ 7,4 km/s;
- aluminum projectile penetration of thin aluminum plate at initial velocity ~ 6,7 km/s;
- shock wave arrival at amplitude ~ 30 GPa at profiled free surface.

Collision of aluminum and titanium plates

- Test problems of different plates collision were used to specify the interaction potentials of different-type clusters, to verify the computational algorithms of averaged physical parameters, to test CDM accuracy.



Collision of aluminum and titanium plates. Distribution of density (left) and pressure (right) at time t = 0.6 μs

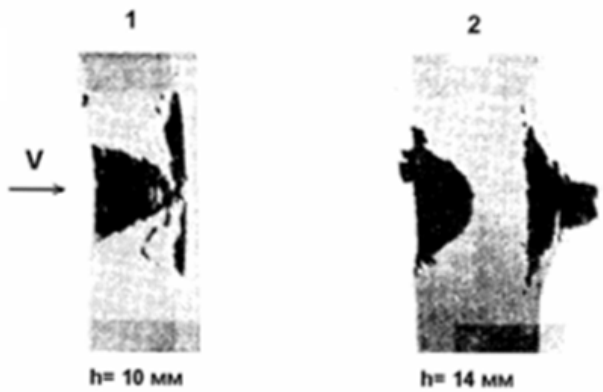
Collision of aluminum and titanium plates

Table - Shock wave initial computation parameters (projectile – titanium) *)

u_0, m/s	Target - Al			Target - Ti		
	P, GPa	u_2, m/s	u_1, m/s	P, GPa	u_2, m/s	u_1, m/s
1000	8.5; 8.3; 8.4	500; 500; 499	500; 500 ; 501	9.95; 9.8; 9.8	424.5; 413; 430	575.5; 587; 570
1500	13.5; 12.8 13.6	750; 749; 751	750; 751; 749	15.8; 15.5; 15.8	640.2; 627; 648	859.8; 873; 852
2000	18.9; 18.1; 19.4	1000; 993; 1001	1000; 1007; 999	22.2; 21.6; 22.9	857; 837; 870	1143; 1163; 1130
3000	31.1; 29.6 33.4	1500; 1493; 1500	1500; 1507; 1500	36.6; 35.8; 39.3;	1295; 1270; 1310	1750; 1730; 1690

*) - black – (p,u)-diagram technique; green – MASTER computation; red – CDM computation

Thick target penetration problems



Глубина проникновения p алюминиевых сферических ударников диаметром ~3,2 мм и массой 0,047 г при скорости удара 7,4 км/с в плоские мишени из сплава 2024-Т3 разной толщины

1-отверстие, d≈2-3 мм.

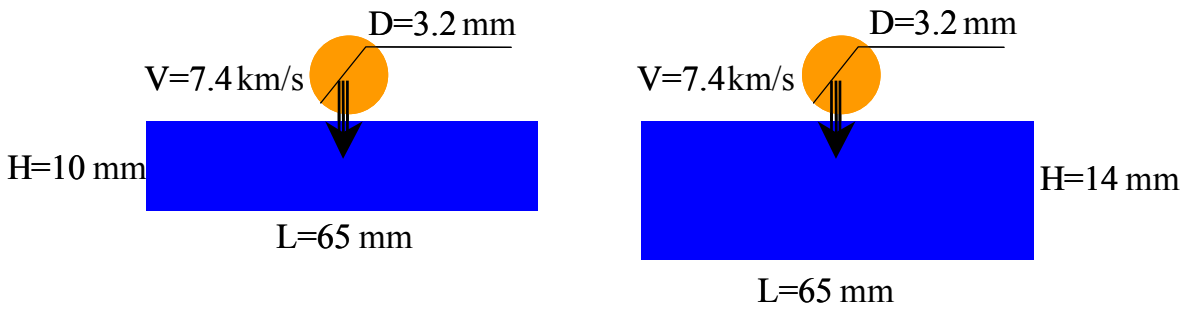
2-кратер, p≈6,9 мм.

ОПЫТНЫЕ ДАННЫЕ

Дж. Геринг. Высокоскоростной удар с инженерной точки зрения
В кн. "Высокоскоростные ударные явления", 1973 г.; с. 468-516.

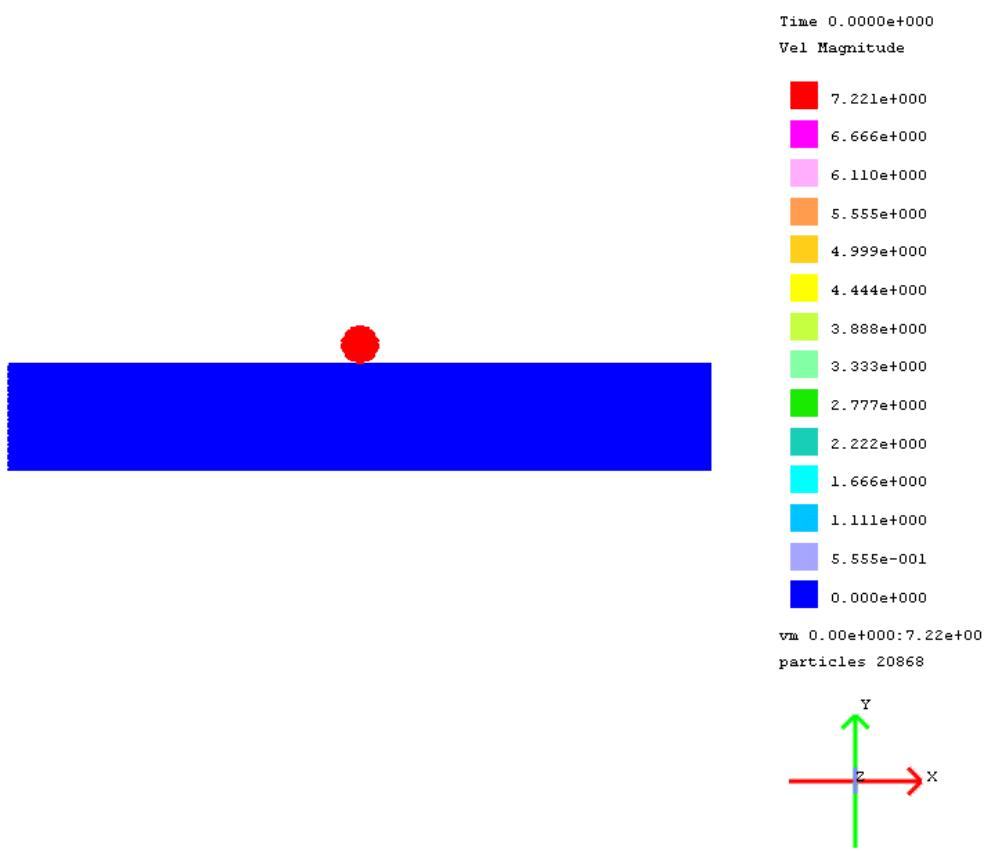
- Gering J. High-velocity impact from the engineering point of view. In: High-velocity impact effects, 1973. P. 468-516.

Thick target penetration problems



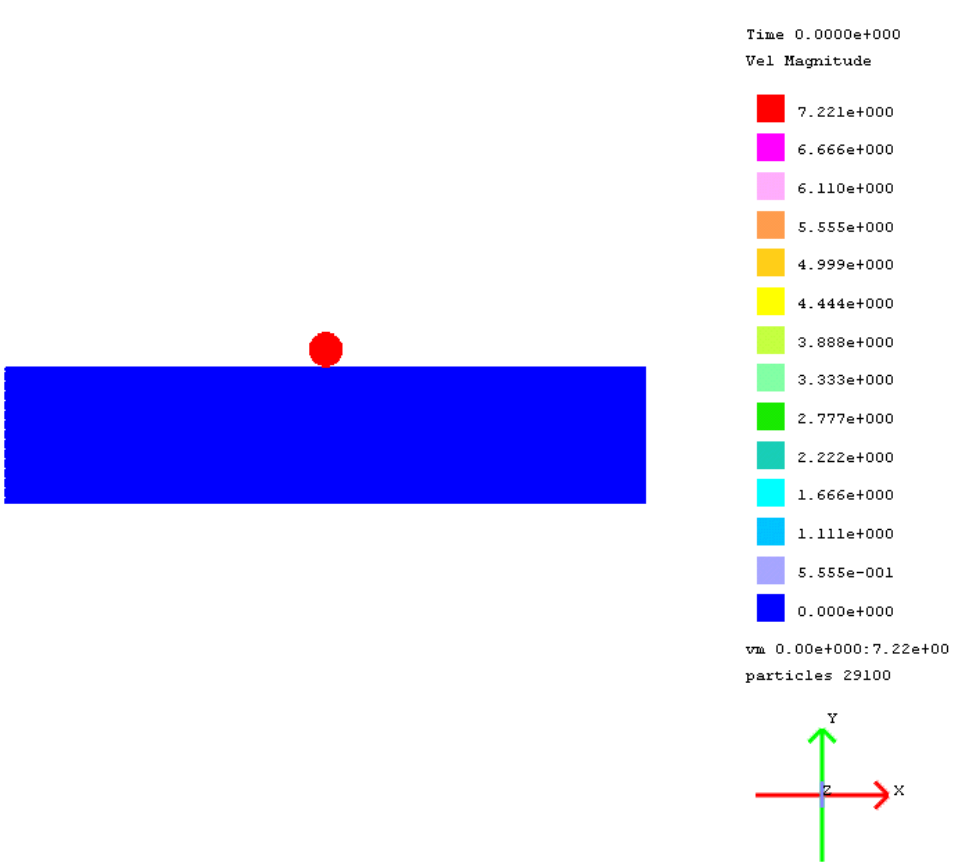
- Two problems of target penetration: Thickness 10 and 14 mm.
- Initial velocity of projectile particles 7,4 km/s, simulated time interval 30 μs, time integration step $0{,}7 \cdot 10^{-9}$ s. Boundary conditions: free upper and lower boundaries; projectile has free boundaries.

Thick target penetration problems



- Computational CDM results.
- Pattern thickness 10 mm
- Potential cut-off radius: 1,15·from 190 μkm

Thick target penetration problems



- Computational CDM results.
- Pattern thickness 14 mm
- Potential cut-off radius: 1,15·from 190 μkm

Thick target penetration problems

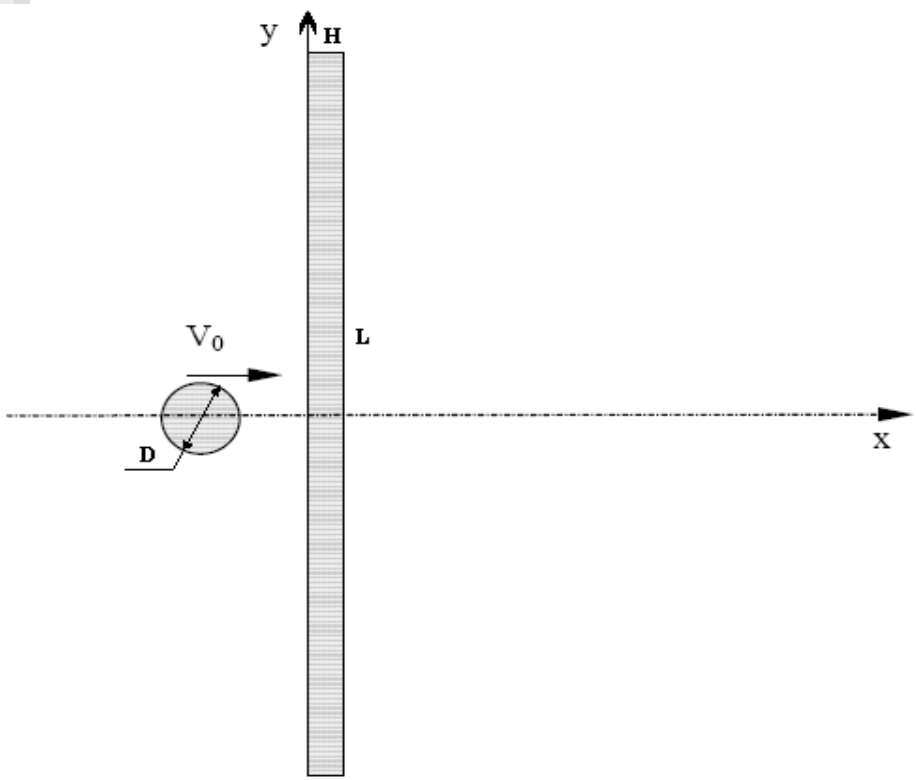
Results can be described in the following way:

- Pattern of fracture corresponds to experimental data for 10 mm thick patterns. Slipping-off of the part of the backside of the plate and its full penetration is observed.
- Slipping-off of the part of the backside of the plate and a ~7 mm deep cratering was observed for the 14 mm thick pattern. However, the fracture behavior behind the crater is of the form of the time accelerating crack. So, we can not speak about the conformity of the computations with experimental results and calculation results using SPH technique.
- In general, the computational results show the necessity of refining model search to describe cluster interaction in strong extension region.

Thin target penetration problem

- Piekutowski A.J. Characteristics of debris clouds produced by hypervelocity impact of aluminum spheres with thin aluminum plates // Int. J. Impact Engng. 1993. Vol.14. P.573-586.

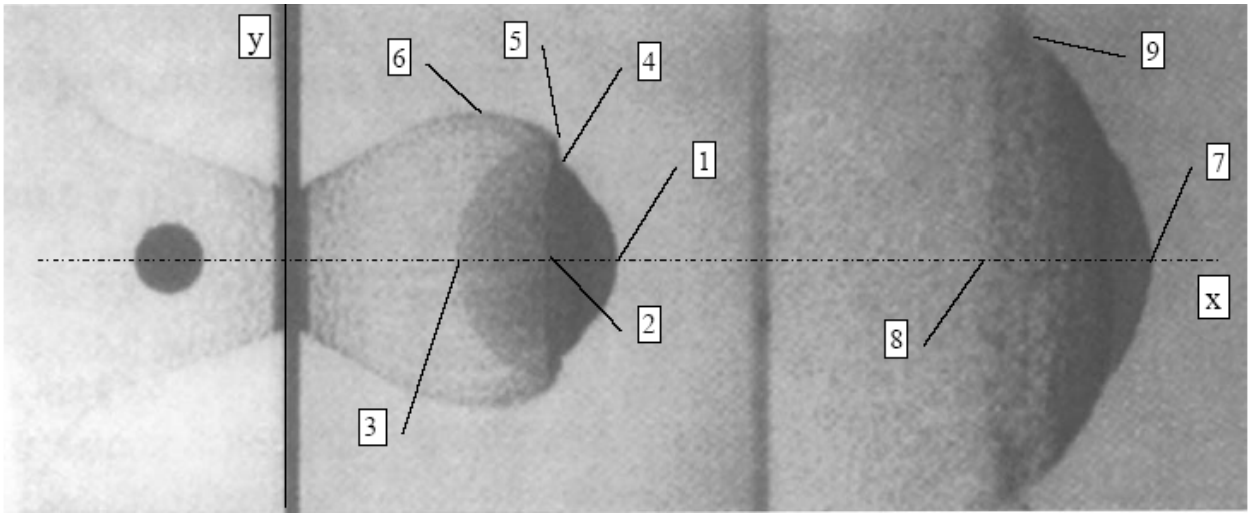
Thin target penetration problem



Basic initial data:

- projectile: aluminum sphere of diameter D=9.53 mm;
- normal impact at velocity V_0=6.71 km/s;
- target: aluminum plate of thickness H=1.549 mm (H/D=0.163).

Thin target penetration problem



The following characteristic points of cloud fragment will be used to compare calculation and experimental data:

- 1 and 7 – front edge of the front element of inner structure;
- 2 and 8 – back edge of the central element of inner structure;
- 3 – back edge of the back element of inner structure;
- 4 and 9 – periphery of the cup-shaped central element of inner structure.

Thin target penetration problem

Coordinates of the characteristic points of fragment cloud (t = 7,2 mks)

Point	x-ray pattern		SPH computation		CDM computation	
	x, cm	y, cm	x, cm	y, cm	x, cm	y, cm
1	4.37	0	4.76	0	4.5	0
2	3.47	0	3.89	0	3.4	0
3	2.28	0	2.39	0	2.4	0
4	3.64	1.33	3.90	1.19	3.4	1.3

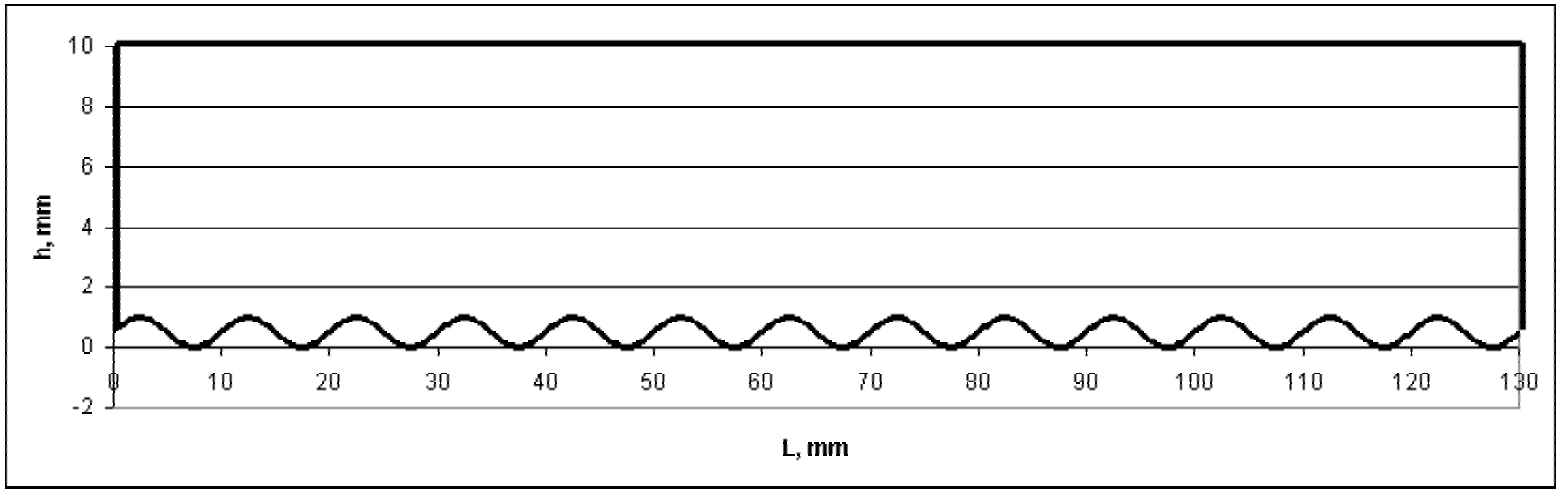
Coordinates of the characteristic points of fragment cloud (t = 19 mks)

Point	x-ray pattern		SPH computation		CDM computation	
	x, cm	y, cm	x, cm	y, cm	x, cm	y, cm
7	11.45	0	12.77	0.00	12	0
8	9.22	0	9.09	0.00	9.2	0
9	9.81	2.89	10.47	2.89	9.2	2.9

Thin target penetration problem

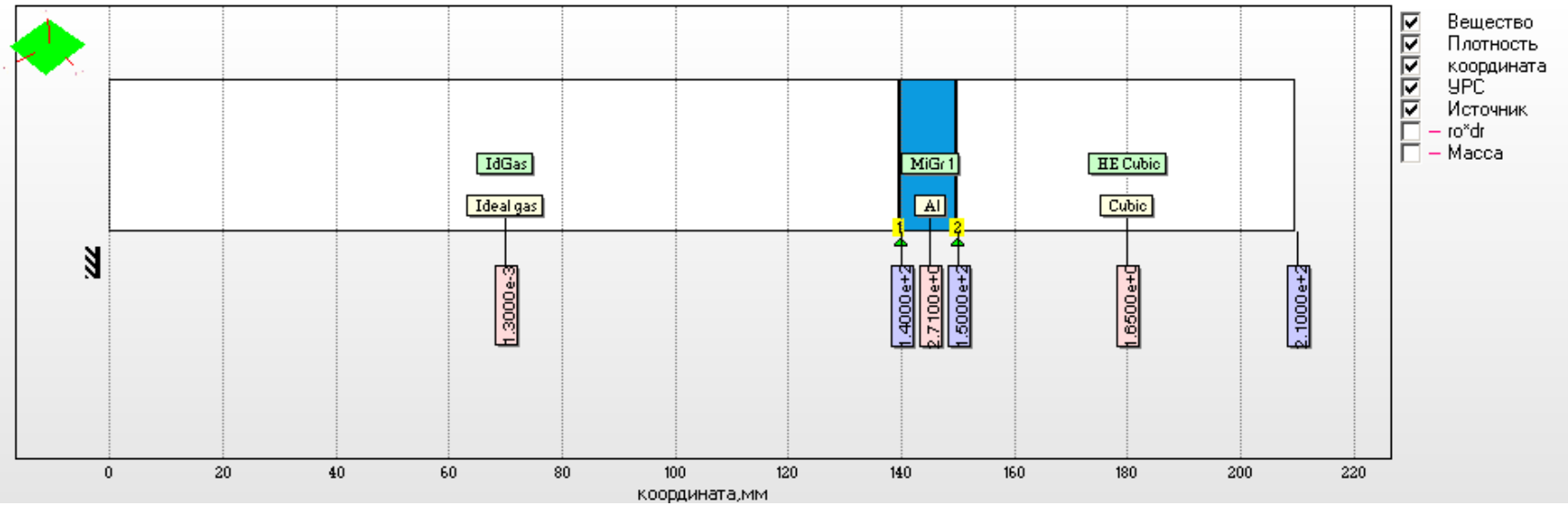
- Difference between computational and experimental results is no more than ~10% for SPH method, as well as for CDM method.
- Fragment field coordinate accuracy of reproduction in CDM method is not worse than in SPH technique.
- Hole diameter computation gives the following results: $D_{эксп}$=17,3 mm, D_{SPH}=18,0 mm, $D_{МКД}$=17,0 mm.
- CDM method gives worse reproduction of inverse fragment separation angle: $Q_{эксп}$~21°; Q_{SPH}~27°; $Q_{МКД}$~39°.

Shock wave arrival at profiled free surface



- The total height of the pattern h=10 mm, the totla length of the pattern L=130 mm.
- Action conditions: shock-wave load was made in the line of h=10 mm (rigid wall at given motion velocity V(t)). The other boundaries are free.

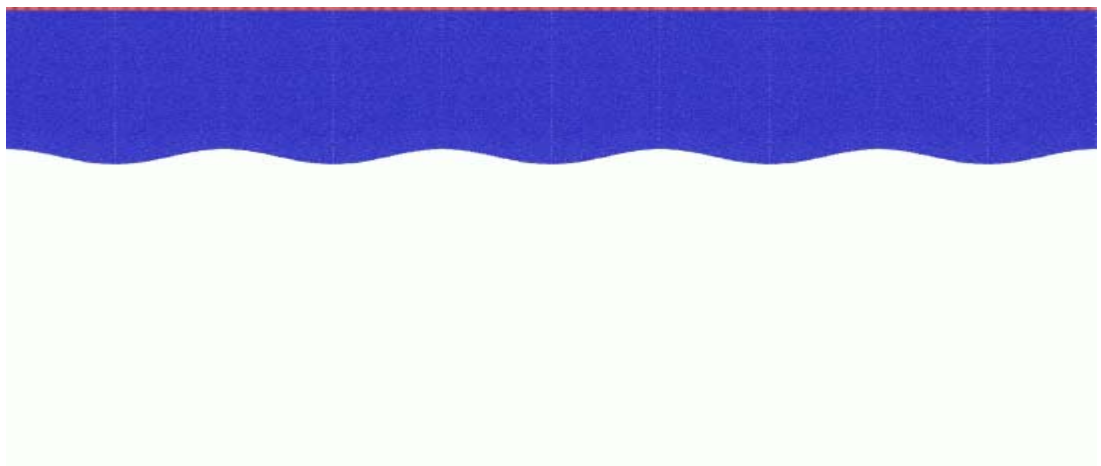
Shock wave arrival at profiled free surface



- 1D gas-dynamic computations were carried out to define wall motion velocity V(t) using MASTER package (www.emerald.sarov.ru). Problem definition corresponded to experimental conditions (aluminum plate thickness 1 cm, explosive charge height 6 cm).

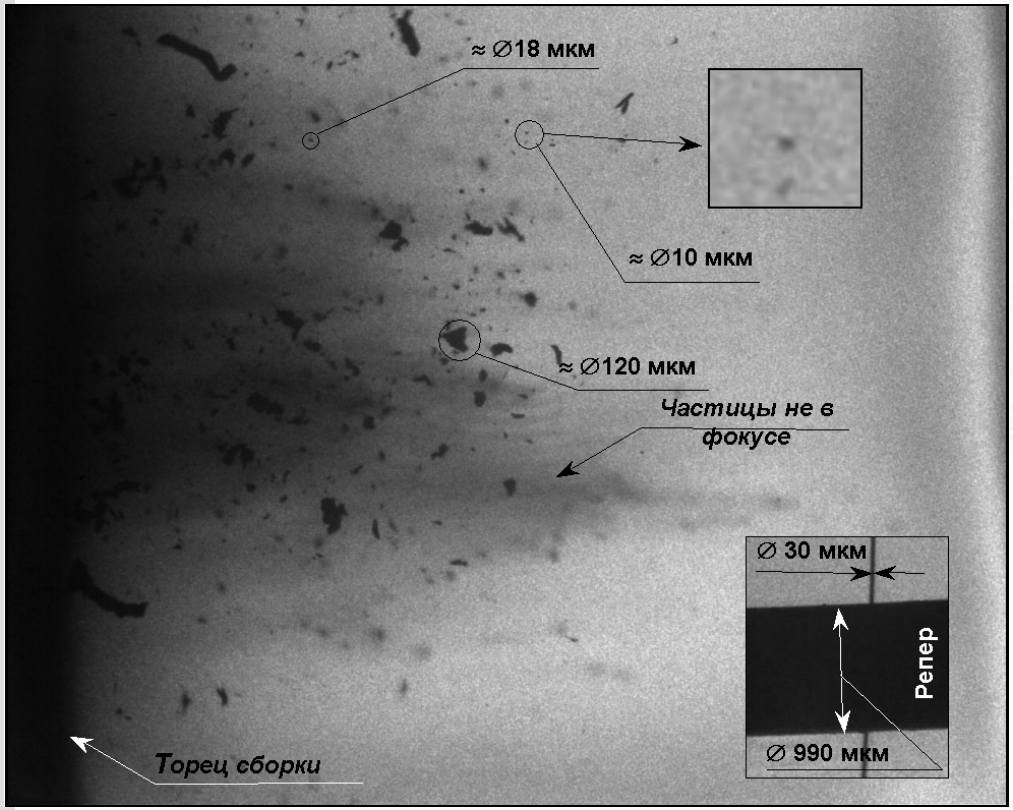
Shock wave arrival at profiled free surface

- The following parameters can defined using computational results:
- time interval used for surface profiling is 2,8÷3,5 μs;
- steady velocity of continuous material is ~3,2 km/s;
- steady velocity of jet flow is~3,7 km/s.
- Computational results are in good agreement with experimental data [V.A. Ogorodnikov, A.A. Sadovoi et al. Jet simulation at shock wave arrival at the profiled free surface. //PMTF. 2006. V.48, №1. P.16-23.

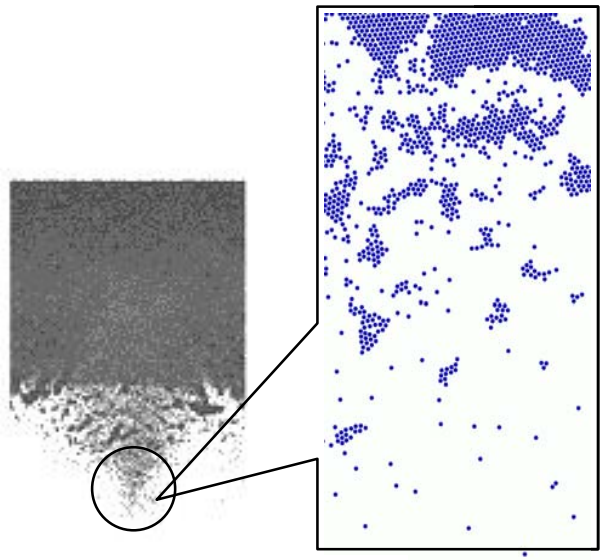


~4 000 000 clustres (1 cluster - 19 μkm); 60 000 steps; 6 μs – physical time.

Shock wave arrival at profiled free surface



Experimental results.



Computational results.

Analogues and CDM software implementation

SPH method

Monaghan J.J. Introduction to SPH. Comp. Phys. Comm. 1987. Vol. 48. P. 89.

Peridynamic method

Silling S.A. Reformulation of elasticity theory for discontinuities and long-range forces. J. Mech. Phys. Sol. 2000. Vol.48, No 1. P. 175.

Particle dynamics method

Krivtsov A.M., Krivtsova H.B. Particle method and its application in deformable solid mechanics. Dalnevostochny matematichesky zhurnal DVO RAS. 2002. V. 3. № 2. P. 254.

Moving cellular automation method

Popov V.L., Psakhie S.G. Theoretical simulation fundamentals of elasto-plastic media using moving cellular automation method. Physical mesomechanics. 2001. V. 4. № 1. P. 17.

Conclusions

- Equations of state used in CDM are generally reproduced from experimental data of shock compression in great number of density points.
- One of the advantages of the method is the possibility of numerical implementation in standard molecular dynamics programs and the possibility to combine CDM with the existed grid gas-dynamic techniques to develop hybrid simulation methods.
- The sufficient advantage of the method is the possibility of simulation of physical processes in a wide range of spatial scale (from micrometer to tens of centimeters) due to the choice of necessary structural cluster.