Russian Supercomputing Days

Moscow, September 25 - 26, 2023

Parallel algorithms

Implementation of dusty gas model based on fast and implicit particle-mesh approach SPH-IDIC in open-source astrophysical code Gadget-2

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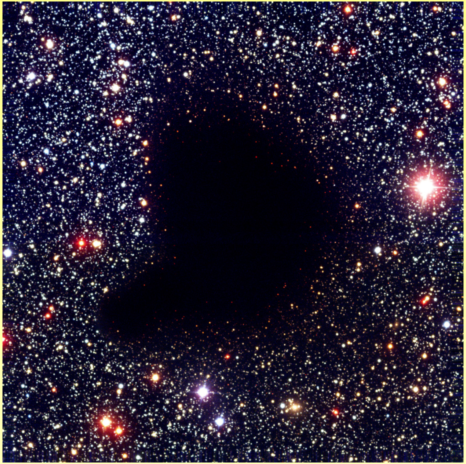
25 September 2023

Introduction – dusty medium



Gas + Dust =
=Two(three, four...)-phase medium

Equations to solve (two phases)

$$\frac{\partial \rho_g}{\partial t} + (\vec{v} \cdot \nabla \rho_g) = -\rho_g \nabla \vec{v}$$

$$\frac{\partial \rho_d}{\partial t} + (\vec{u} \cdot \nabla \rho_d) = -\rho_d \nabla \vec{u}$$

$$\frac{\partial (\rho_g \vec{v})}{\partial t} + \nabla \cdot \left(\rho \vec{v} \cdot \vec{v} - p\hat{I}\right)^T = \nabla \cdot \Pi(\nu) + D_{gas}$$

$$\frac{\partial (\rho_d \vec{u})}{\partial t} + \nabla \cdot (\rho_d \vec{u} \cdot \vec{u})^T = D_{dust}$$

$$\frac{\partial S}{\partial t} = \frac{1}{2} \frac{\gamma - 1}{\rho^{\gamma-1}} \nabla \cdot (\vec{v} \cdot \Pi(\nu))$$

$$p = (\gamma - 1)\rho_g \epsilon, \qquad S = \frac{p}{\rho^\gamma},$$

ρ_g — gas density

$\vec{v}$ — gas velocity

ρ_d — dust density

$\vec{u}$ — dust velocity

p — gas pressure

$D \sim \frac{\vec{v}-\vec{u}}{t_{stop}}$ — drag force

ϵ — SIE, S — entropy

$\Pi(\nu)$ — numerical viscosity

γ — adiabatic parameter

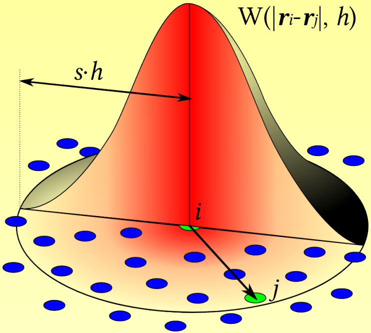
Smooth particle hydrodynamics

Approximation of any parameters:

$$f(\mathbf{r}) = \int\limits_{\Omega} f(\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}')dx' \approx \int\limits_{\Omega} f(\mathbf{r}')W(|\mathbf{r}-\mathbf{r}'|,h)d\mathbf{r}' \approx \sum_{j=1} m_j \frac{f(\mathbf{r}_j)}{\rho_j} W(|\mathbf{r}-\mathbf{r}_j|,h)$$

Kernel M_4

$$W(\mathbf{r},h) = \alpha \begin{cases} 1 - \frac{3}{2}q^2 + \frac{3}{4}q^3, & 0 \le q \le 1, \\ \frac{1}{4}(2-q)^3, & 1 < q \le 2, \\ 0, & 2 < q, \end{cases} \qquad q = \frac{|\mathbf{r}|}{h}$$



Monaghan, J.J., Annual Review of Astronomy and Astrophysics, 1992

Monaghan&Kocharyan approach

Drag force on gas:

$$D_a^n = -\lambda \sum_j m_j \frac{K_{aj}^n}{\rho_a^n \rho_j^n} \frac{(\vec{v}_a^n - \vec{v}_j^n) \cdot (\vec{r}_j^n - \vec{r}_a^n)}{|\vec{r}_j^n - \vec{r}_a^n|^2 + \eta \overline{h_{aj}^n}^2} |\vec{r}_j^n - \vec{r}_a^n| W(r_{ja}^n, h_a^n)$$

Drag force on dust:

$$D_i^n = \lambda \sum_b m_b \frac{K_{bi}^n}{\rho_b^n \rho_i^n} \frac{(\vec{v}_b^n - \vec{v}_i^n) \cdot (\vec{r}_i^n - \vec{r}_b^n)}{|\vec{r}_i^n - \vec{r}_b^n|^2 + \eta \overline{h_{bi}^n}^2} |\vec{r}_i^n - \vec{r}_b^n| W(r_{ib}^n, h_i^n)$$

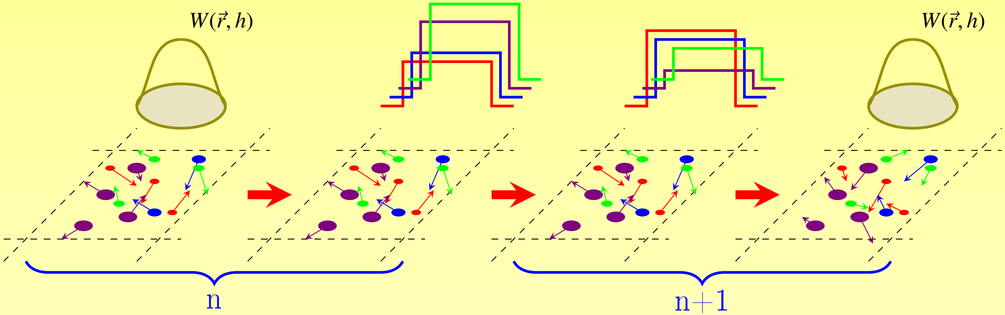
Dependence on dust parameters:

$$K_{aj}^n = \frac{\rho_j^n \rho_a^n c^n}{s \rho_s} = \frac{\rho_j^n}{t_{stop}^n}$$

Monaghan, J. J., Kocharyan, A., Computer Physics Communications, 1995

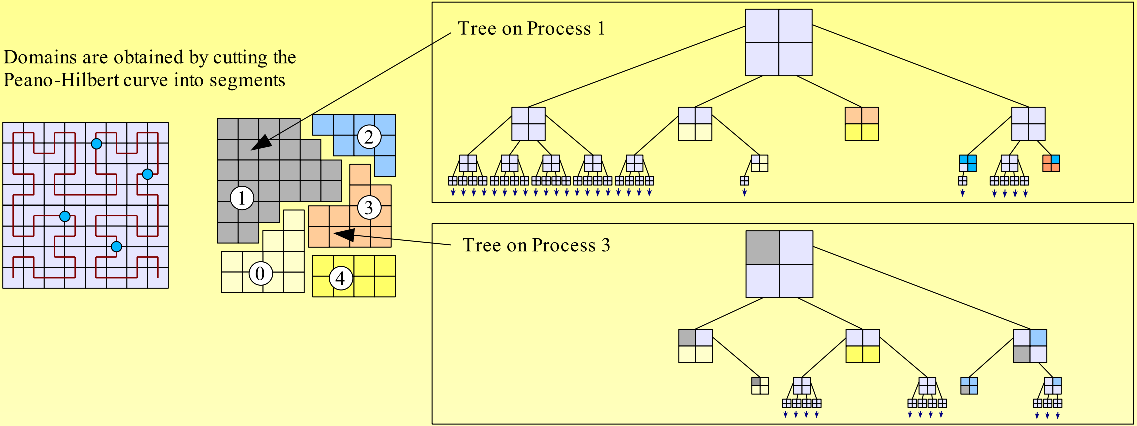
SPH + Implicit Drag-In-Cell method

IDIC: *Stoyanovskaya+, Astronomy and Computing, 2018*, *Stoyanovskaya+, Journal of Computational Physics, 2021*



Idea of IDIC: Velocities → Average velocities → New average velocities → New velocities

SPH cosmological simulations, Tree-code for approximation of gravity

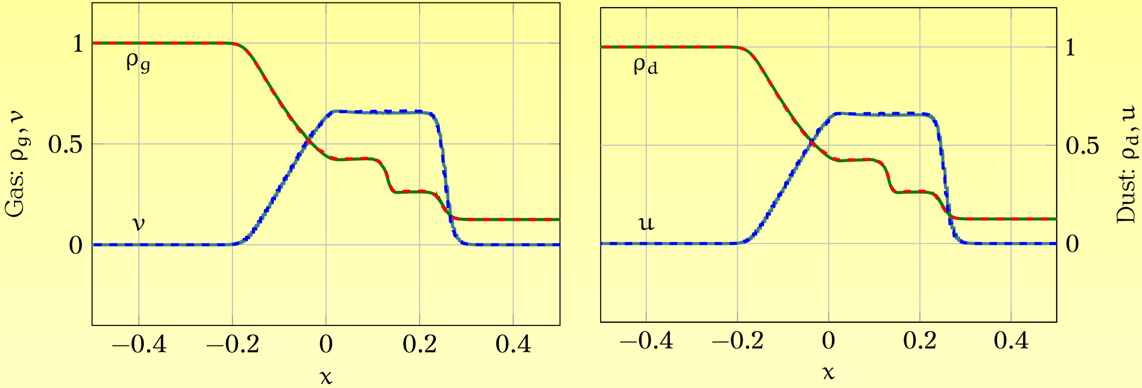


Springel, MNRAS, 2005

Sod's tube problem: constant m vs. constant N

Initial conditions

$$(\rho_g, p, v, \epsilon) = \begin{cases} (1.0, 1.0, 0, 2.5) & x < 0 \\ (0.125, 0.1, 0, 2.0) & x > 0 \end{cases} \qquad \gamma = 1.4 \qquad t_{stop} \sim 10^{-4}$$

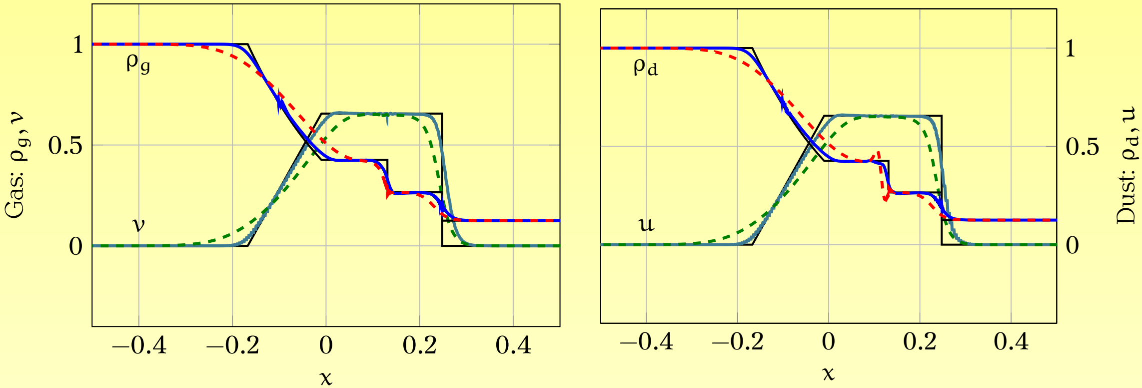


SPH-IDIC: $h = 2 \times 10^{-2}$, $\Delta t = 10^{-3}$, solid: m=const, dashed: N=const

Sod's tube problem: MK vs. IDIC, small t_{stop}

Initial conditions

$$(\rho_g, p, v, \epsilon) = \begin{cases} (1.0, 1.0, 0, 2.5) & x < 0 \\ (0.125, 0.1, 0, 2.0) & x > 0 \end{cases} \qquad \gamma = 1.4 \qquad t_{stop} \sim 10^{-3}$$

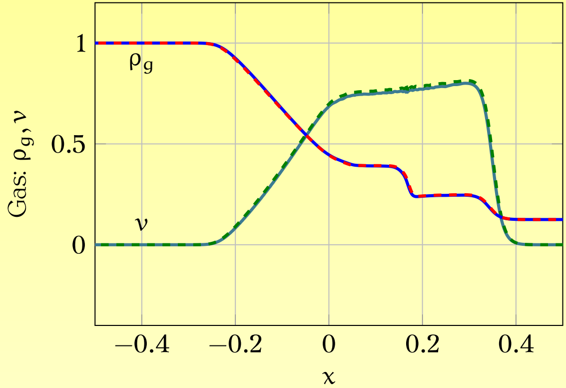


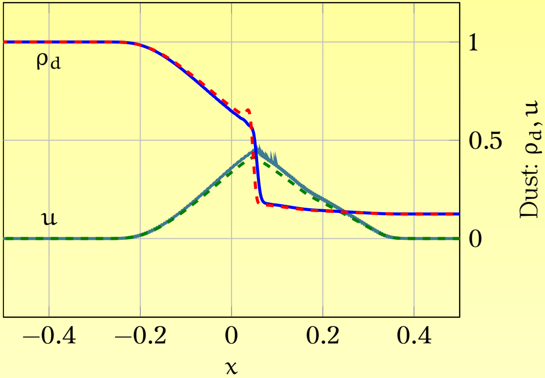
SPH: $h = 2 \times 10^{-2}$, solid: IDIC ($\Delta t = 10^{-3}$), dashed: MK ($\Delta t = 10^{-4}$)

Sod's tube problem: MK vs. IDIC, medium t_{stop}

Initial conditions

$$(\rho_g, p, v, \epsilon) = \begin{cases} (1.0, 1.0, 0, 2.5) & x < 0 \\ (0.125, 0.1, 0, 2.0) & x > 0 \end{cases} \qquad \gamma = 1.4 \qquad t_{stop} \sim 10^{-1}$$



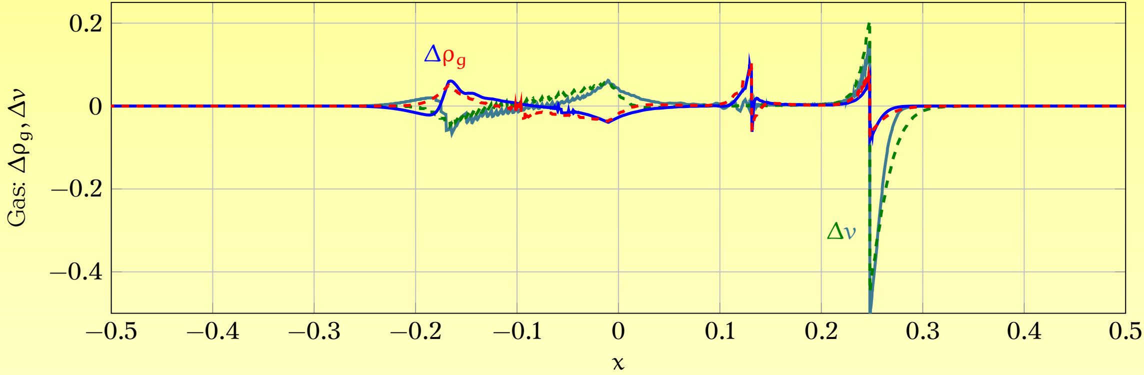


SPH: $h = 2 \times 10^{-2}$, $\Delta t = 10^{-3}$, solid: IDIC, dashed: MK

Sod's tube problem, IDIC: variable h vs. h=const

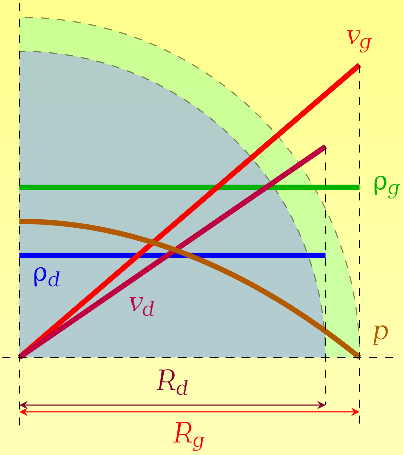
Initial conditions

$$(\rho_g, p, v, \epsilon) = \begin{cases} (1.0, 1.0, 0, 2.5) & x < 0 \\ (0.125, 0.1, 0, 2.0) & x > 0 \end{cases} \qquad \gamma = 1.4 \qquad t_{stop} \sim 10^{-3}$$



SPH: $\Delta t = 10^{-3}$, solid: variable h, dashed: h=const

Expansion of Dusty ball into vacuum – 3D: problem and solution

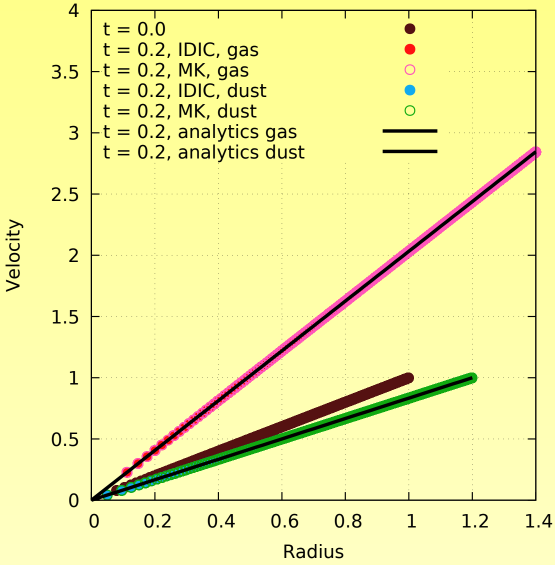


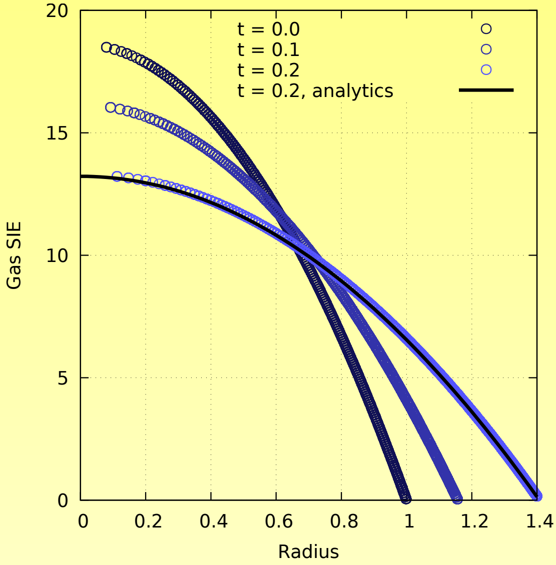
Stoyanovskaya+, Fluids, 2021

Analytical solution:

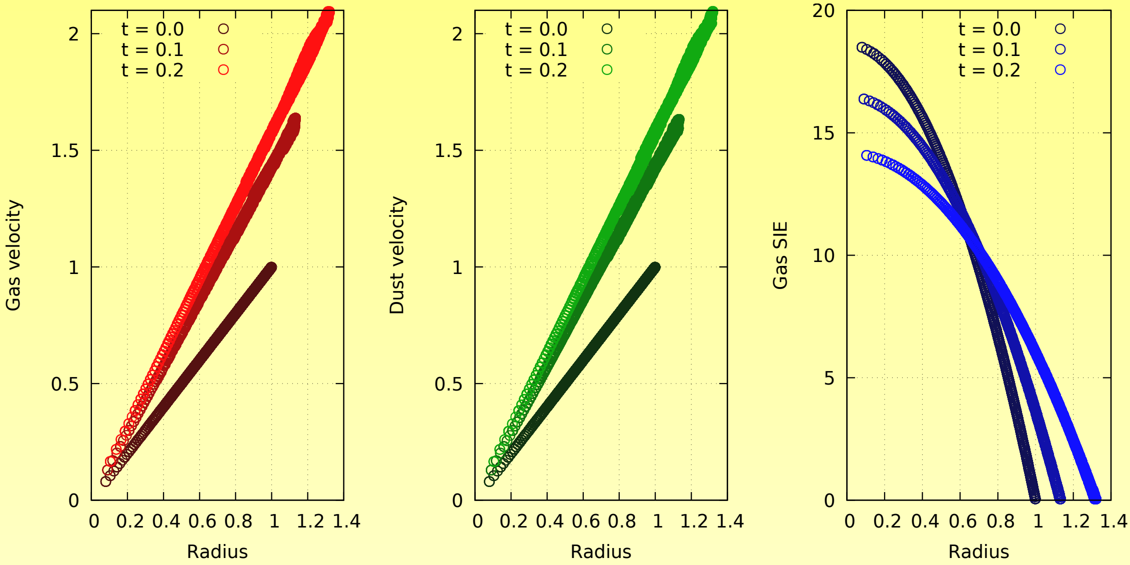
$$
\begin{cases}
\dfrac{dR_\mathrm{g}}{dt} = \dot{R}_\mathrm{g}, \qquad \dfrac{dR_\mathrm{d}}{dt} = \dot{R}_\mathrm{d} \\
\dfrac{d\dot{R}_\mathrm{d}}{dt} = \dfrac{R_\mathrm{d}}{t_\mathrm{stop}}\left(\dfrac{\dot{R}_\mathrm{g}}{R_\mathrm{g}} - \dfrac{\dot{R}_\mathrm{d}}{R_\mathrm{d}}\right) \\
\dfrac{d\dot{R}_\mathrm{g}}{dt} = 2(\gamma-1)C^* R_\mathrm{g}^{2-3\gamma} - \dfrac{1}{t_\mathrm{stop}}\dfrac{M_\mathrm{d}R_\mathrm{g}^4}{M_\mathrm{g}R_\mathrm{d}^3}\left(\dfrac{\dot{R}_\mathrm{g}}{R_\mathrm{g}} - \dfrac{\dot{R}_\mathrm{d}}{R_\mathrm{d}}\right) \\
\dfrac{\partial E}{\partial t} = -3\dfrac{(\gamma-1)E\dot{R}_\mathrm{g}}{R_\mathrm{g}}, \qquad p = (\gamma-1)\rho_g E(t)\left(1 - \dfrac{r^2}{R_\mathrm{g}^2}\right) \\
v_g(r,t) = \dot{R}_\mathrm{g}\dfrac{r}{R_\mathrm{g}}, \qquad v_d(r,t) = \dot{R}_\mathrm{d}\dfrac{r}{R_\mathrm{d}} \\
\rho_\mathrm{g}(t) = \dfrac{3M_\mathrm{g}}{4\pi R_\mathrm{g}^3(t)}, \qquad \rho_\mathrm{d}(t) = \dfrac{3M_\mathrm{d}}{4\pi R_\mathrm{d}^3(t)}
\end{cases}
$$

Dusty ball – 3D: large relaxation time

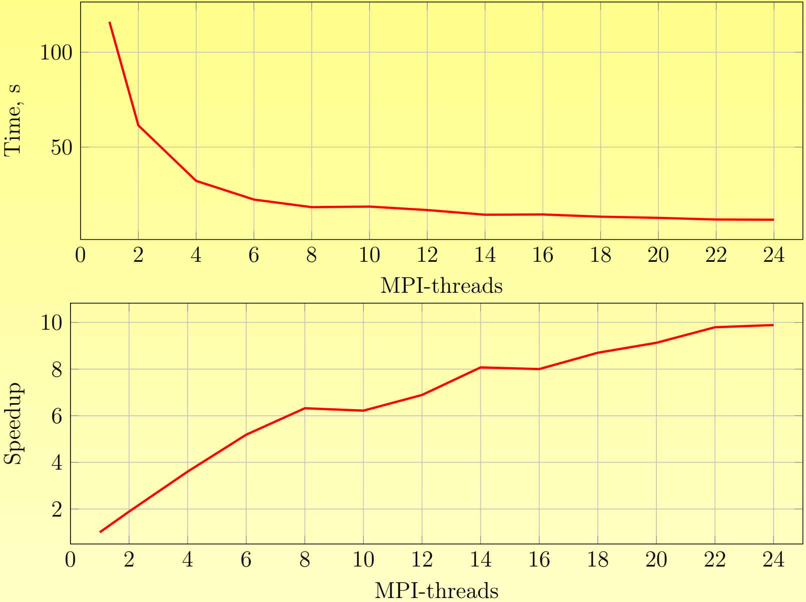




Dusty ball – 3D: small relaxation time



Parallelization of IDIC: 12th Gen Intel(c) Core ™i9-12900K × 16



Results

- Implementation of the SPH-IDIC method using the Gadget-2 package was verified
- 1D and 3D calculations show significant advantage of SPH-IDIC over MK-scheme when small t_{stop}
- SPH-IDIC is parallelizable algorithm, speedup ~ 10 with 24 threads

I‘m grateful for your attention :-)

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colab.ws: R-36020-0CB4F-JB45S

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