# A Treecode Algorithm for Regularized Particle Interactions

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## outline

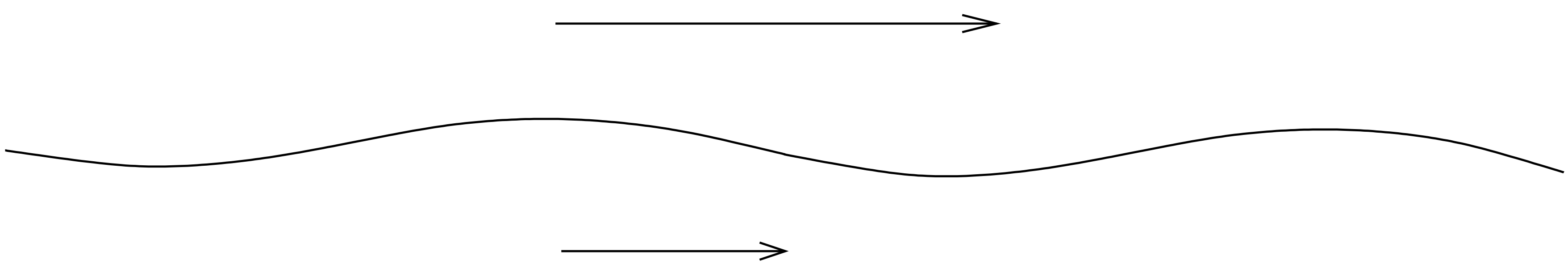
1. Kelvin-Helmholtz instability
2. vortex sheet model
3. regularized particle method
4. treecode algorithm
5. vortex ring simulations

# Kelvin-Helmholtz instability

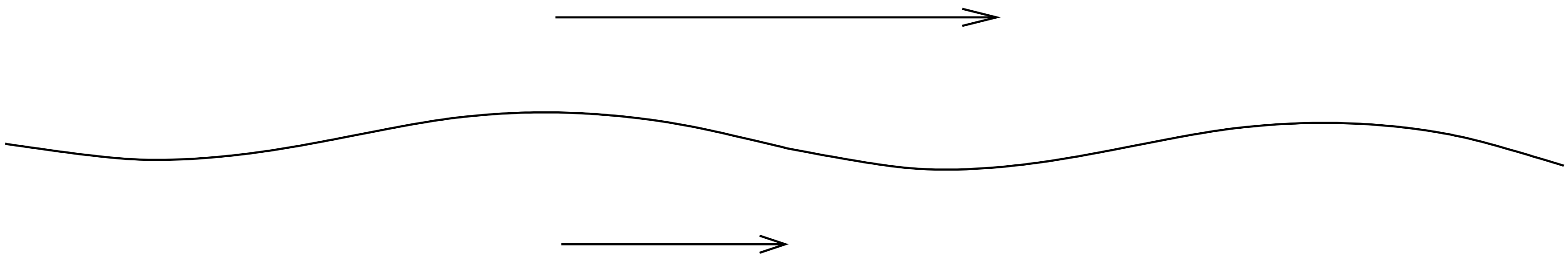
Roberts, Dimotakis & Roshko (1985)

"An Album of Fluid Motion" , Van Dyke

# vortex sheet model



# vortex sheet model



linear stability

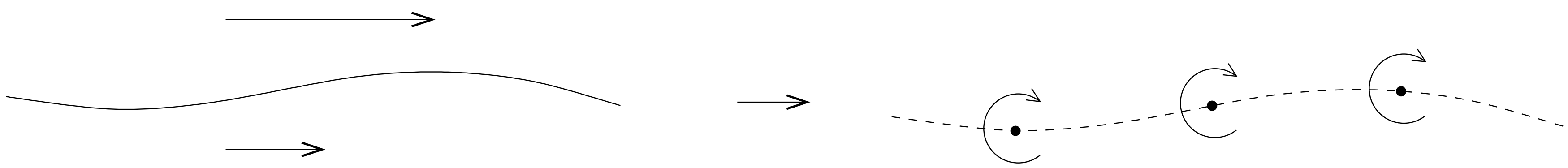
$\exp(st + ikx)$ , $s \sim k$ $\Rightarrow$ ill-posed IVP

Birkhoff-Rott equation

$$z(\Gamma, t) \quad , \quad \frac{\overline{\partial z}}{\partial t} = \text{pv}\int_a^b K(z - \tilde{z}\,)\, d\tilde{\Gamma} \quad , \quad K(z) = \frac{1}{2\pi i z}$$

Moore (1979) : singularity formation

# regularized particle method



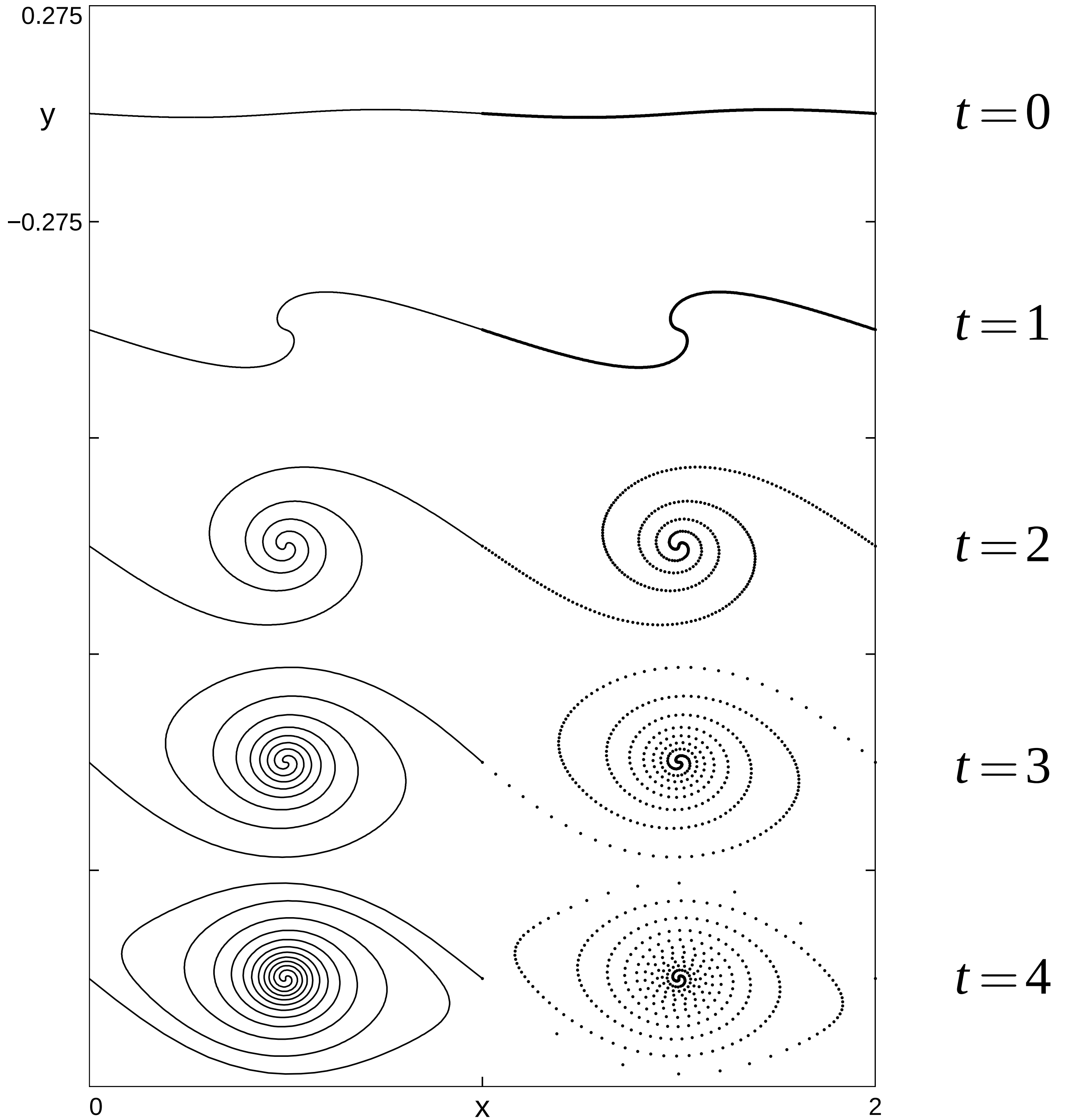
$$z(\Gamma,t) \;\rightarrow\; z_j(t)\;,\; j=1,\ldots,N$$

$$\overline{\frac{dz_j}{dt}} = \sum_{k=1}^{N} K_\delta(z_j - z_k)\,\Gamma_k \quad , \quad K_\delta(z) = \frac{1}{2\pi i z}\cdot\frac{|z|^2}{|z|^2+\delta^2}$$

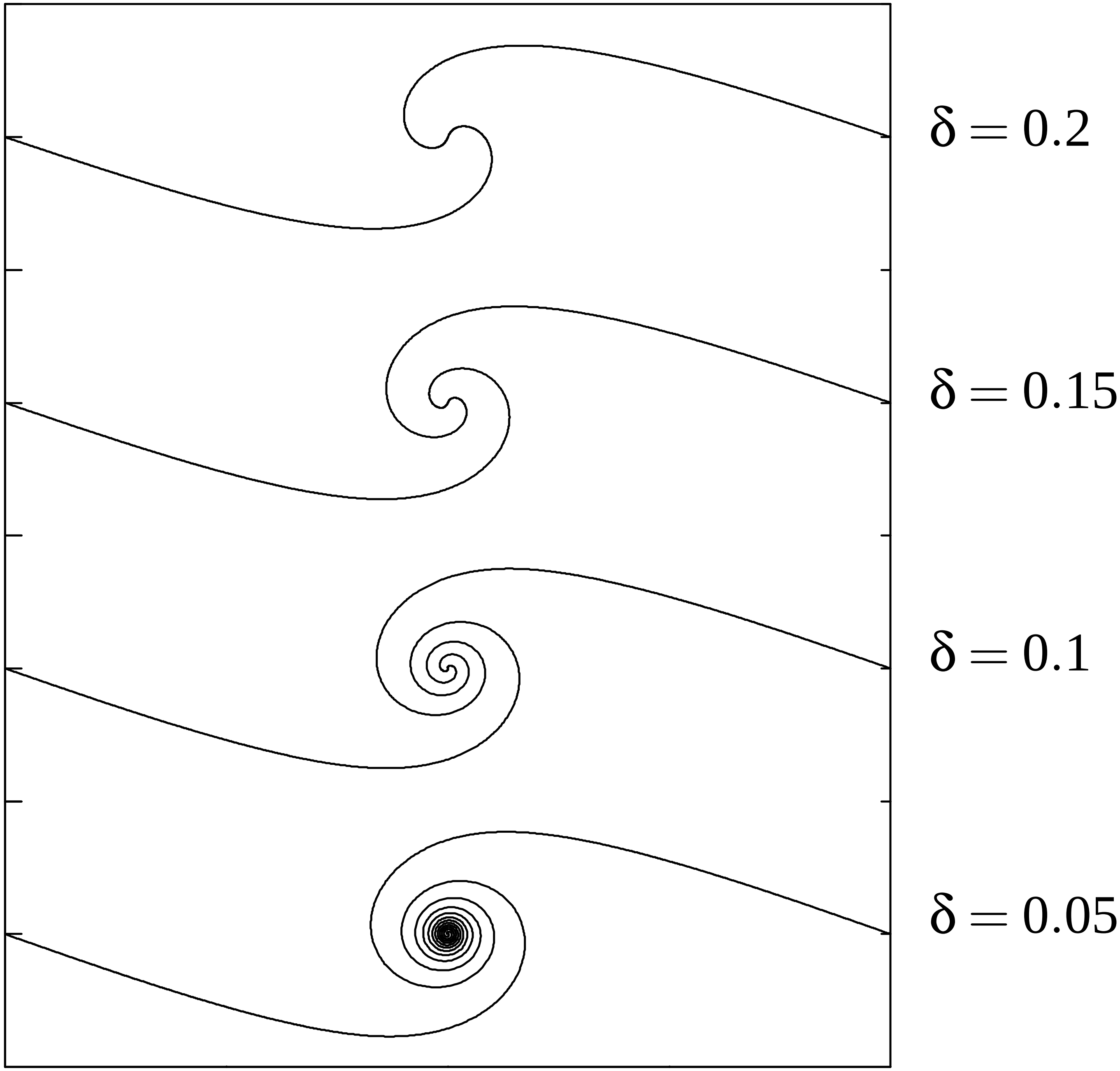
$\delta$ : smoothing parameter

vortex-blob method , Chorin & Bernard (1973)

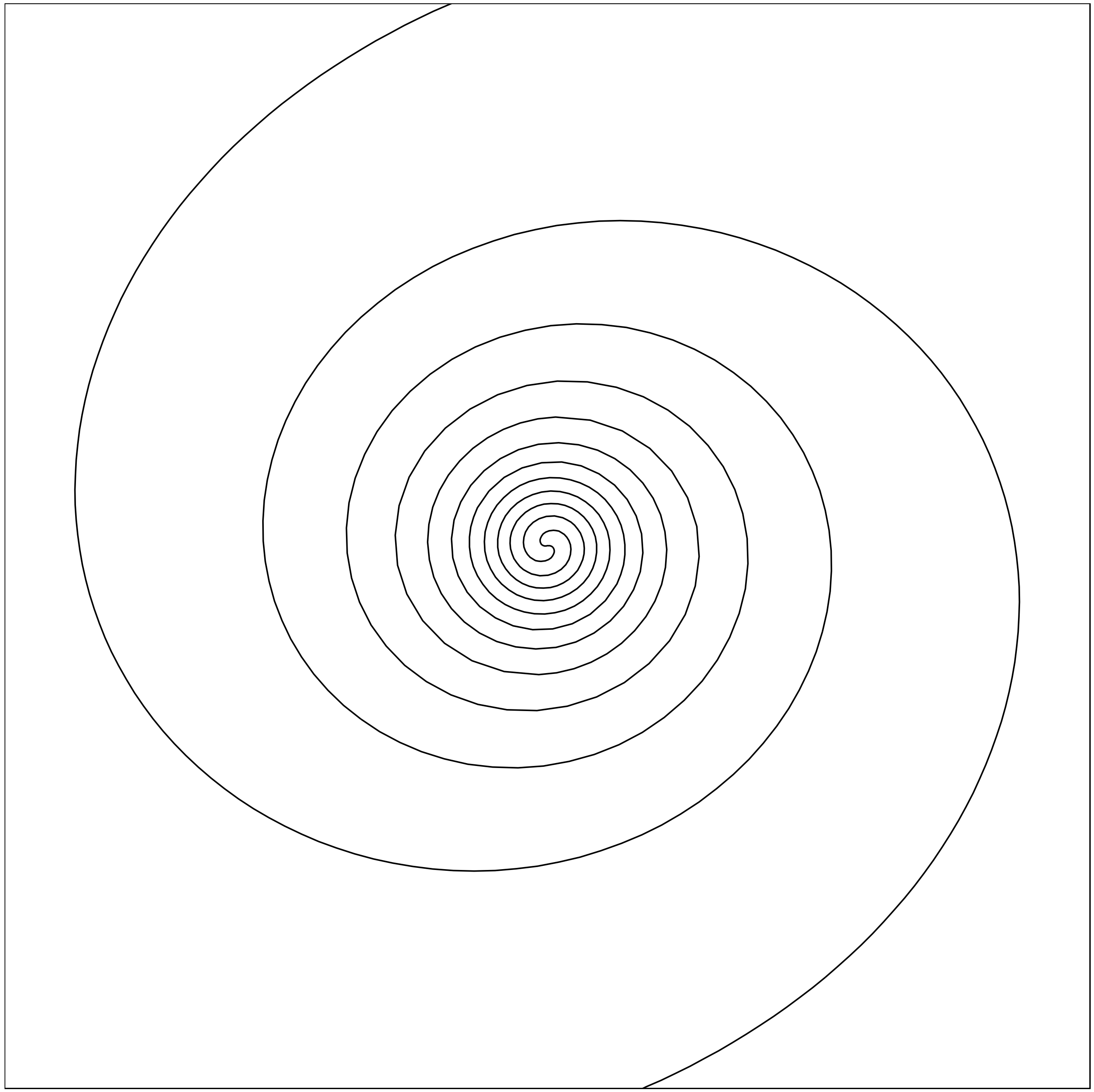
$\delta = 0.25$ , $N = 400$ Krasny (1986)



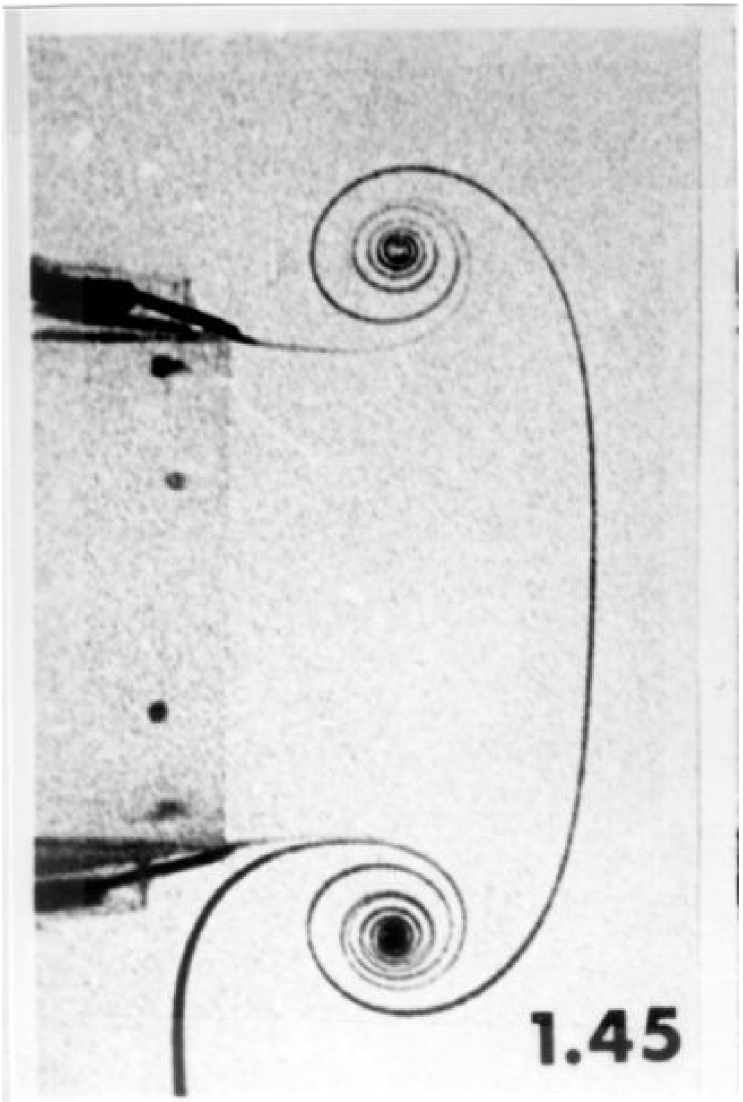
$t = 1\ ,\ \delta \to 0$



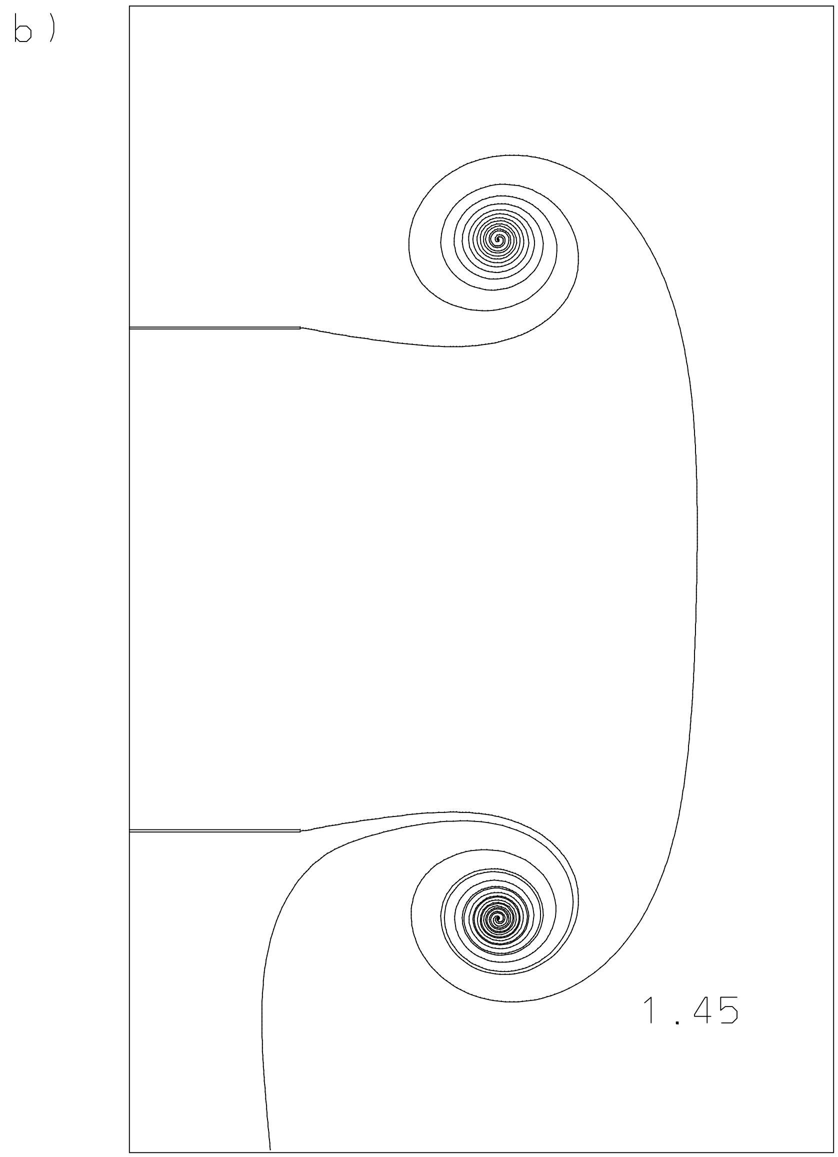
closeup , $\delta = 0.05$



# comparison : experiment / simulation

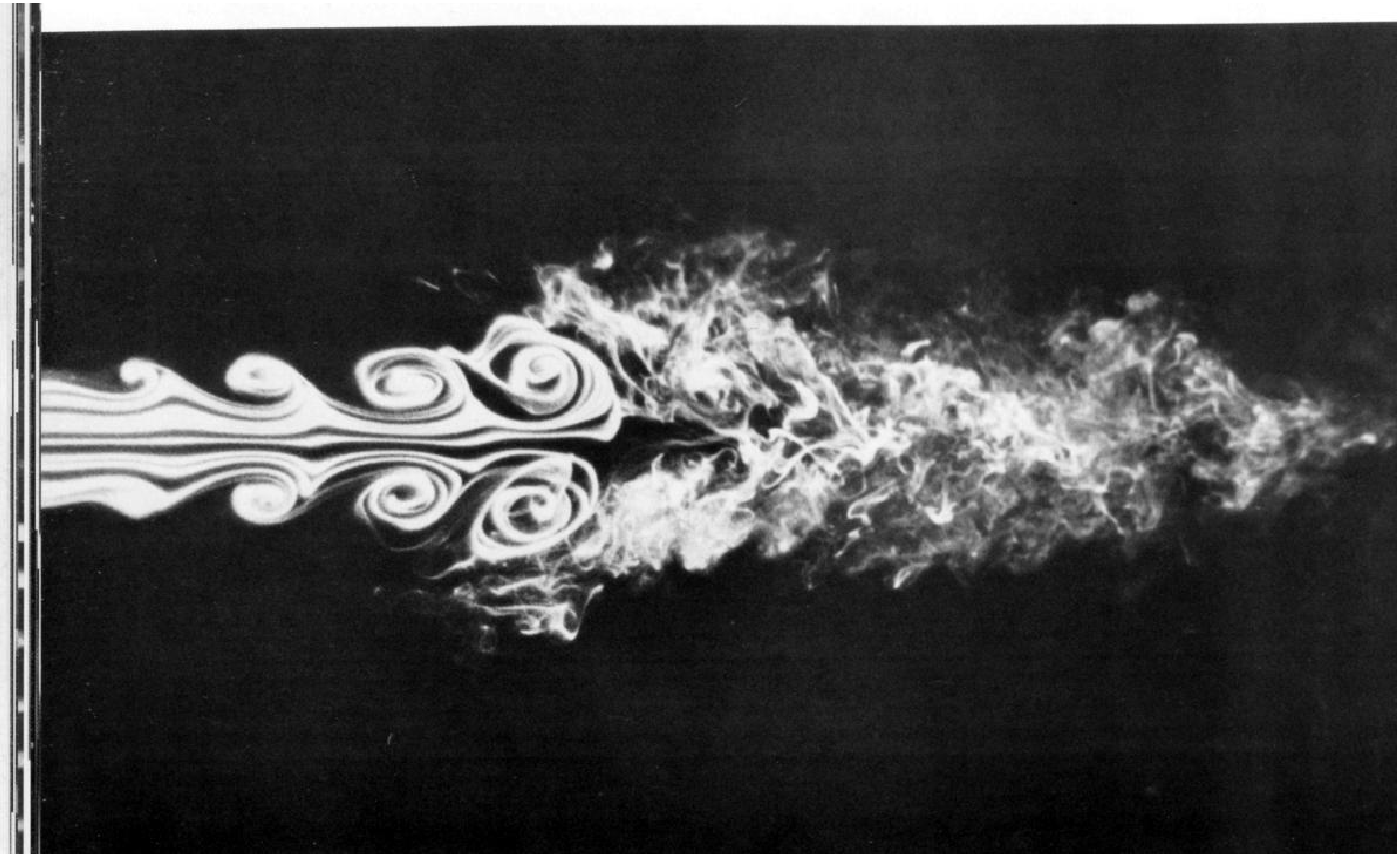



Didden (1979)



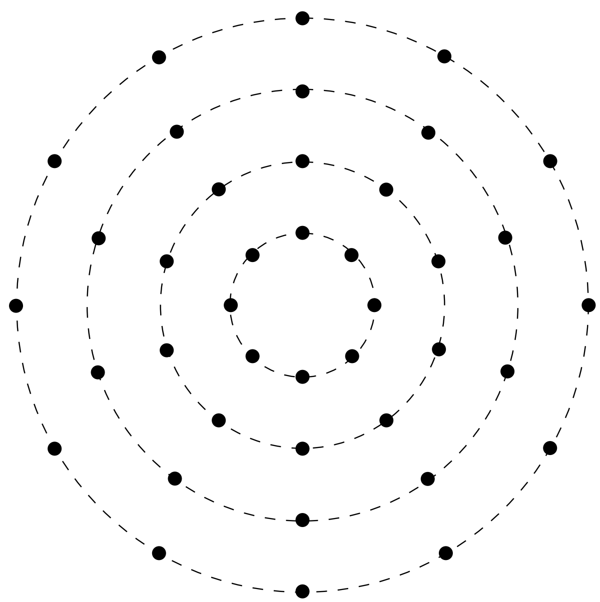

Nitsche & Krasny (1994)

# <u>3D instability in a circular jet</u> (Drubka & Nagib)



# vortex sheet model in 3D flow

vortex ring : $x(\Gamma, \theta, t) \rightarrow x_i(t)$ , $i = 1, \ldots, N$



$$\frac{dx_i}{dt} = \sum_{j=1}^{N} K_\delta(x_i, x_j) \times w_j$$

$$K_\delta(x, y) = -\frac{x - y}{4\pi(|x-y|^2 + \delta^2)^{3/2}}$$ : Biot-Savart kernel

$$\frac{dx_i}{dt} = \sum_{j=1}^{N} K_\delta(x_i, x_j) \times w_j$$ : $N$-body problem

direct summation : $O(N^2)$

particle-particle

treecode algorithm : $O(N \log N)$

Barnes & Hut (1986)

particle-cluster

monopole approximation

one-pass , divide-and-conquer

fast multipole method : $O(N)$

Greengard & Rokhlin (1987)

cluster-cluster

multipole approximation, spherical harmonics

two-pass , interaction list , multipole-to-local transformation , ...

## obstacle

$$K_\delta(x,y) = -\frac{x-y}{4\pi(|x-y|^2+\delta^2)^{3/2}}$$ : nonharmonic

## solution

Draghicescu & Draghicescu (1995)

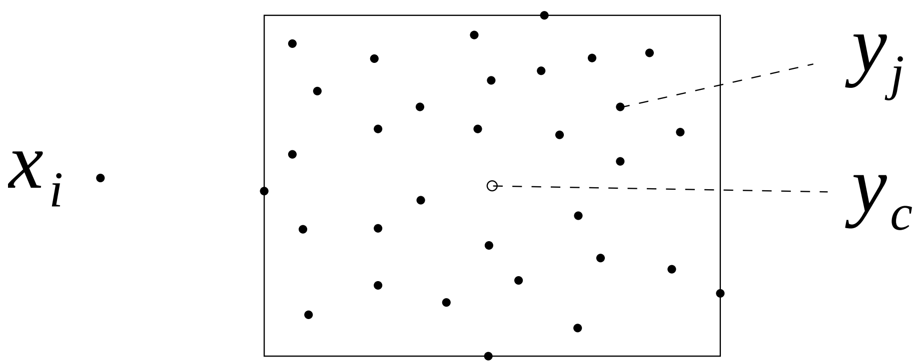
Taylor expansion in Cartesian coordinates

particle-cluster treecode

adaptive techniques

# particle-cluster treecode

$$\sum_{j=1}^{N} K_\delta(x_i, x_j) \times w_j = \sum_{c} \sum_{j=1}^{N_c} K_\delta(x_i, y_j) \times w_j$$




$$\sum_{j=1}^{N_c} K_\delta(x_i, y_j) \times w_j = \sum_{j=1}^{N_c} K_\delta(x_i, y_c + (y_j - y_c)) \times w_j$$

$$= \sum_{j=1}^{N_c} \sum_{k} \frac{1}{k!} D_y^k K_\delta(x_i, y_c)(y_j - y_c)^k \times w_j$$

$$\approx \sum_{||k||<p} \frac{1}{k!} D_y^k K_\delta(x_i, y_c) \times \sum_{j=1}^{N_c} (y_j - y_c)^k w_j$$

## Taylor coefficients

$$K_\delta(x,y) = -\frac{x-y}{4\pi(|x-y|^2+\delta^2)^{3/2}} = -\nabla_y \phi_\delta(x,y)$$

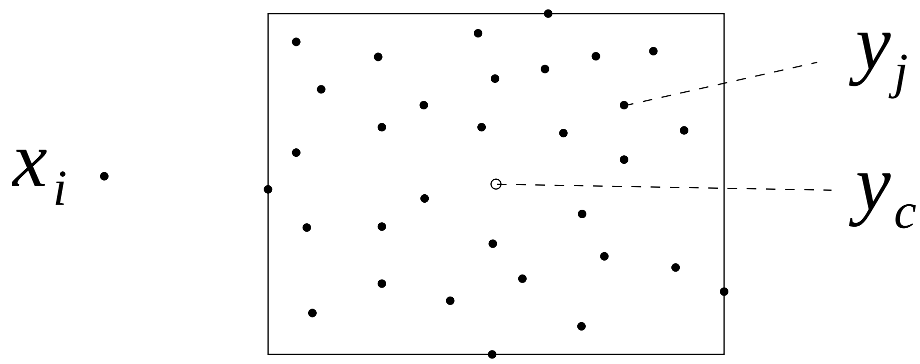
$$\phi_\delta(x,y) = \frac{1}{4\pi(|x-y|^2+\delta^2)^{1/2}}$$ : Plummer potential

## recurrence relation

define : $a_k = \frac{1}{k!} D_y^k \phi_\delta(x,y)$ , $R^2 = |x-y|^2 + \delta^2$

$$a_k = \frac{2||k||-1}{||k||\,R^2} \sum_{i=1}^{3} (x_i - y_i) a_{k-e_i} - \frac{||k||-1}{||k||\,R^2} \sum_{i=1}^{3} a_{k-2e_i}$$

## multipole acceptance criterion : MAC



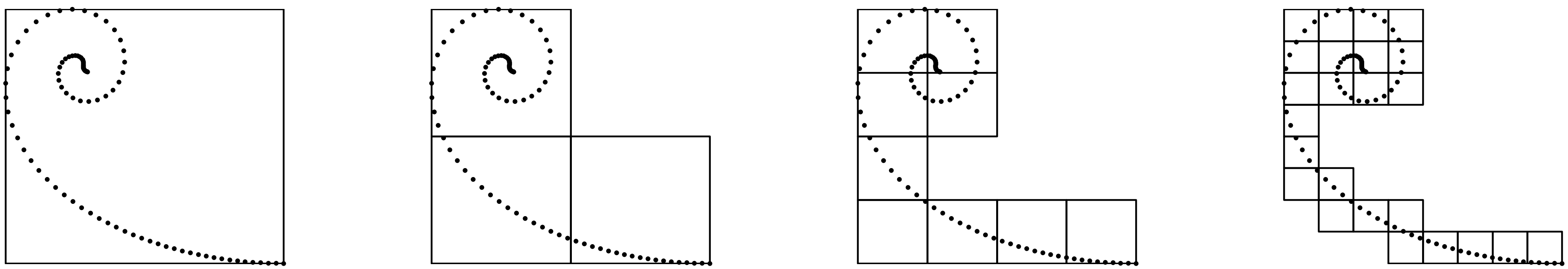

$$\frac{M_p(c)}{4\pi R^{p+1}} \leq \varepsilon$$ : accuracy parameter

$$M_p(c) = \sum_{j=1}^{N_c} |y_j - y_c|^p |w_j| \quad , \quad R^2 = |x-y|^2 + \delta^2$$

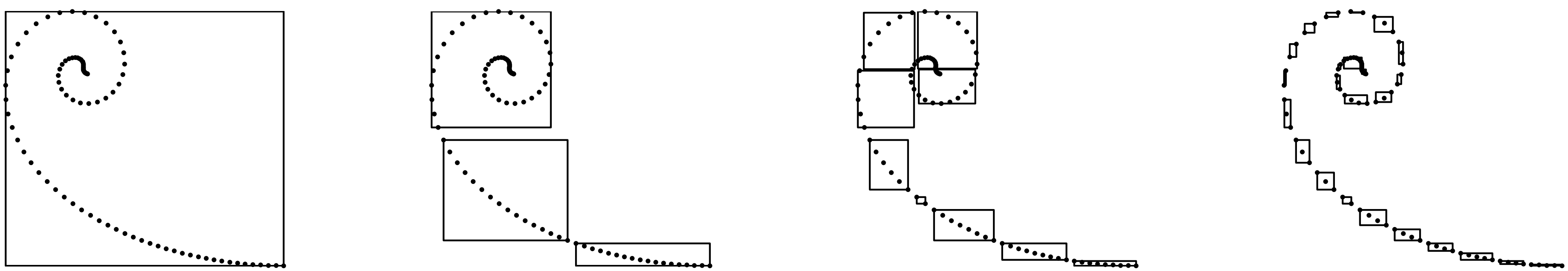
# tree structure

## standard scheme

level 1 level 2 level 3 level 4



## present scheme



# code structure

input particle data

$x_i \ , \ w_i \ , \ i = 1, \ldots, N$

input treecode parameters

$\varepsilon \ , \ p \ , \ N_0$

construct tree

compute particle velocities

for $i = 1 : N$

**compute-velocity**$(x_i, root)$

end

function **compute-velocity**($x$, $c$)

if MAC is satisfied

    compute Taylor coefficients

    compute moments of cluster $c$ (if needed)

    compute particle-cluster velocity by Taylor approximation

else

    if $c$ is a leaf

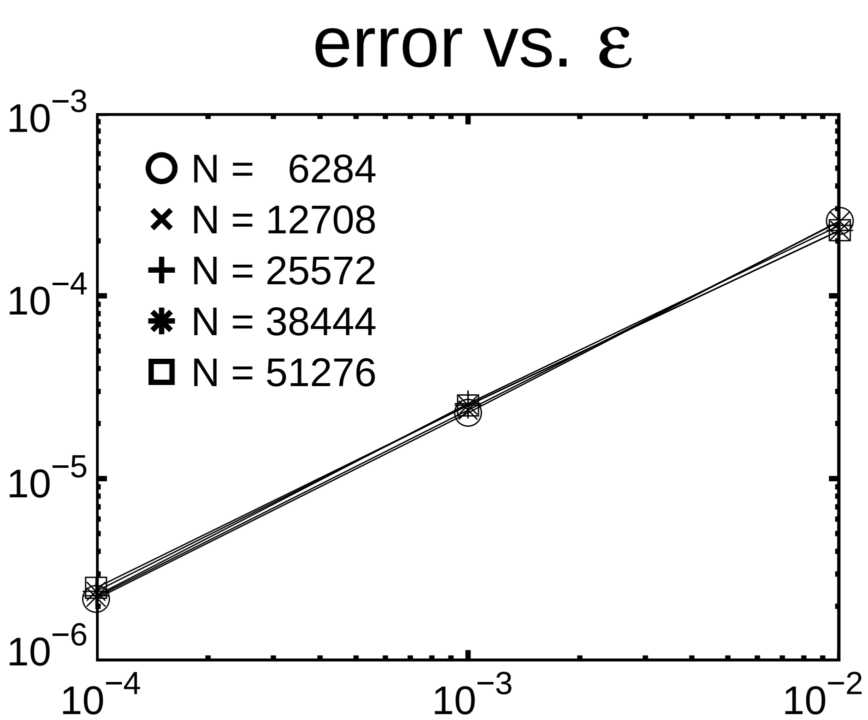
        compute particle-cluster velocity by direct summation

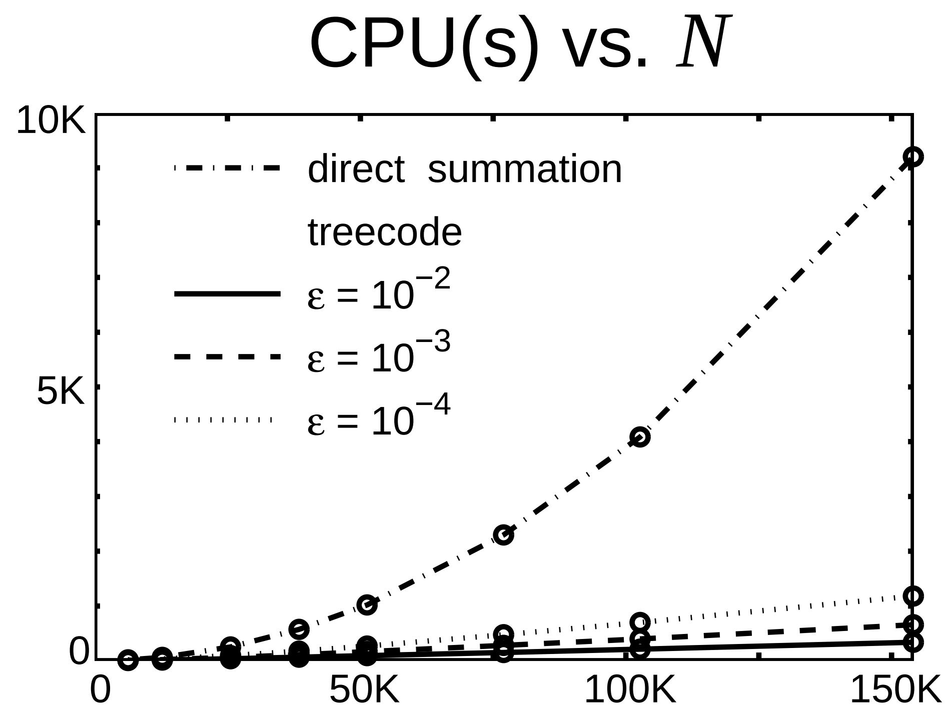
    else

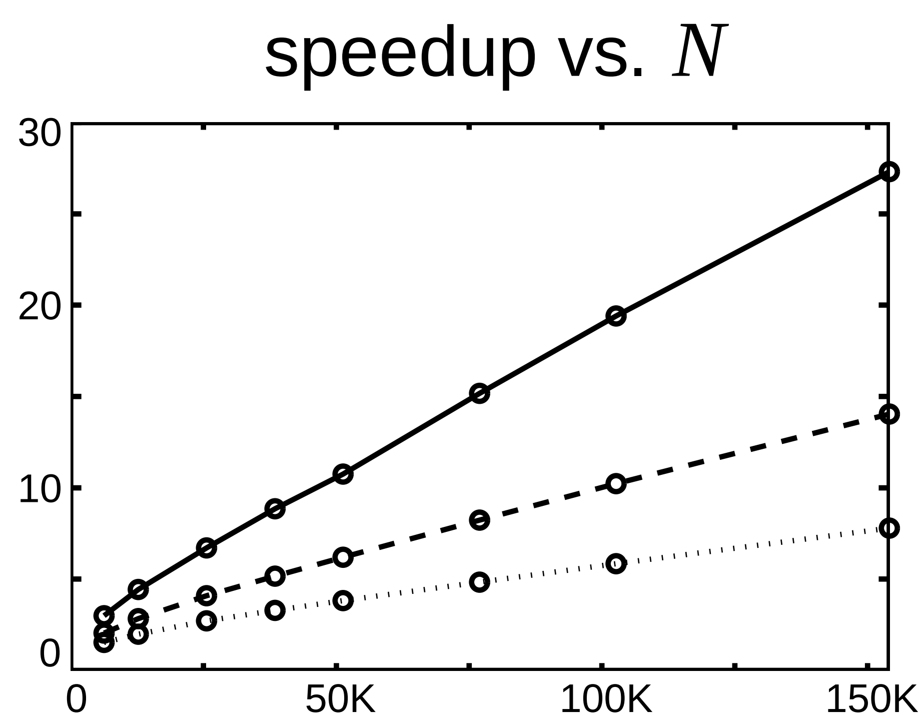
        for each child $\widehat{c}$ of cluster $c$

                **compute-velocity**($x$, $\widehat{c}$)

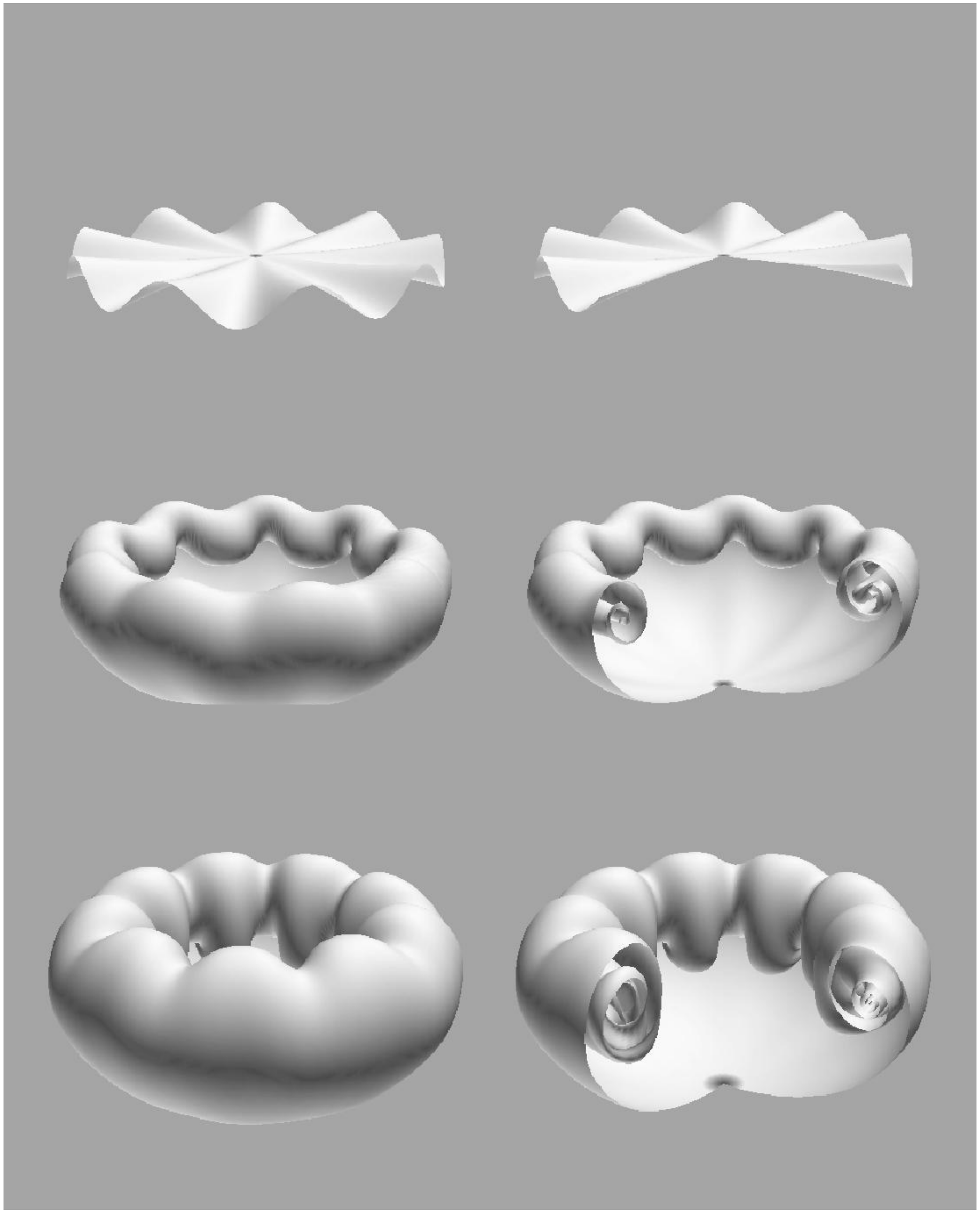
# test case


error vs. ε
10−3
10−4
10−5
10−6
10−4
10−3
10−2
N = 6284
N = 12708
N = 25572
N = 38444
N = 51276

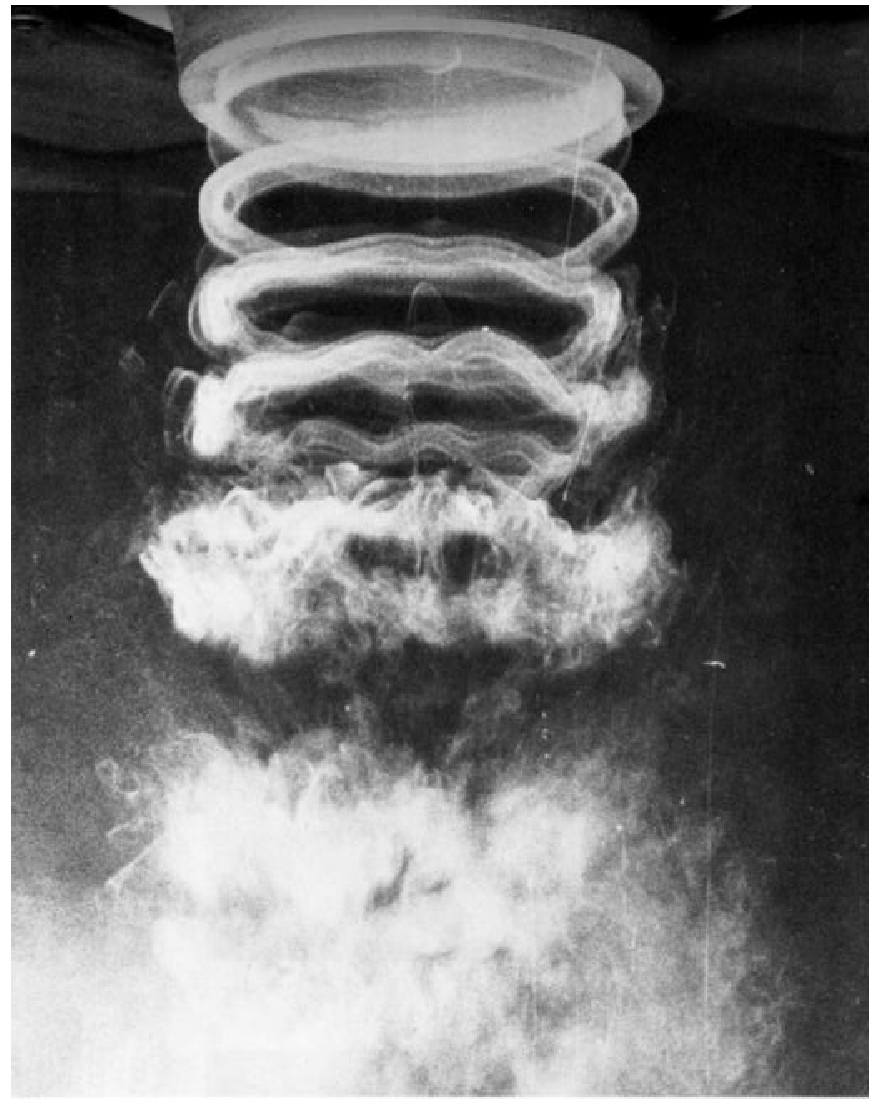

CPU(s) vs. N
10K
5K
0
0
50K
100K
150K
direct summation
treecode
ε = 10−2
ε = 10−3
ε = 10−4


speedup vs. N
30
20
10
0
0
50K
100K
150K

treecode simulation
$N = 10K \rightarrow 200K$



experiment
Wille & Michalke



## molecular dynamics   with Zhong-Hui Duan , Hans Johnston

1. general power law potential

$$\phi(x) = \frac{1}{|x|^{\nu}}$$

2. periodic BC , Ewald summation

$$\phi(x) = \frac{\text{erfc}(\alpha x)}{|x|}$$

## plasma dynamics   with Andrew Christlieb

1. 1D virtual cathode

2. magnetically confined electron column

## papers

fluid dynamics (with Keith Lindsay)

J. Comput. Phys. 172 (2001)

molecular dynamics (with Zhong-Hui Duan)

J. Comput. Chem. 22 (2001)

J. Chem. Phys. 113 (2000)

http://www.math.lsa.umich.edu/∼krasny

## codes

www.cgd.ucar.edu/oce/klindsay

www.cs.uakron.edu/∼zduan

www.math.lsa.umich.edu/∼hansjohn

www.math.lsa.umich.edu/ christli/treecode.html

## bottom line

particle-cluster treecode , Cartesian coordinates , adaptivity