Computational Physics

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Differential equations for Astrophysics
Lund Observatory
FYSN33 - Lecture 1

Summary of this part of the course

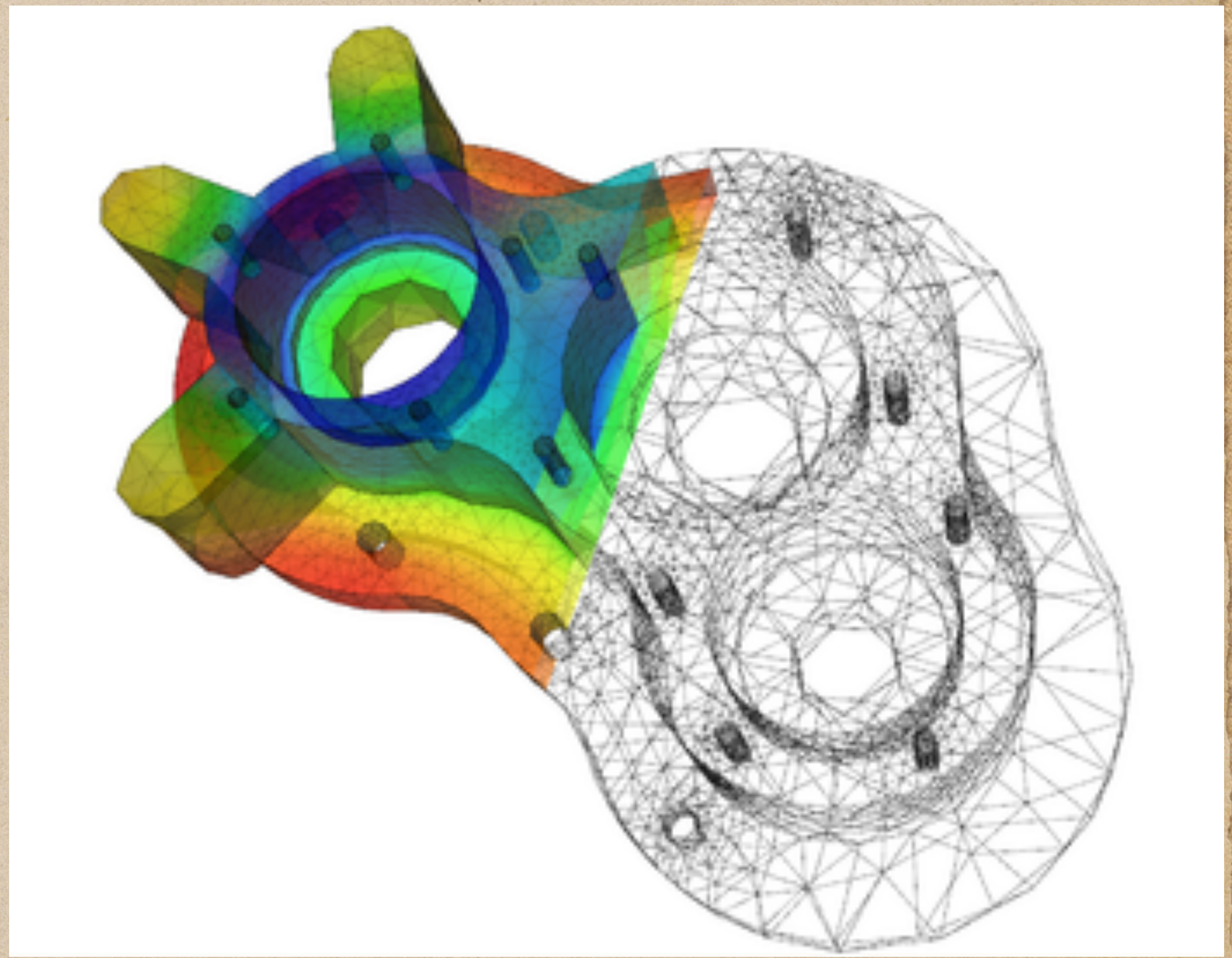
- General introduction
- In this course we will implement the Navier-Stokes equations of hydrodynamics
- We will do this using Smoothed Particle Hydrodynamics (SPH)
- You will firstly solve Sod's Shock Tube problem in 1D - this is a standard test for hydrodynamical codes
- You will then apply the same method (by including gravitation) to simulate and collide two gas giant planets

Differential Equations in Physics

In mathematics, a differential equation is an equation that relates one or more functions and their derivatives.

In physical applications:

- the functions generally represent physical quantities
- the derivatives often represent their rates of change or spatial changes.
- the differential equation defines a relationship between the two.



Visualisation of heat transfer in a pump casing, created by solving the heat equation. From wikipedia.

Why are differential equations used for expressing physical laws?*

Physical laws are a set of rules followed by a system. They are used to explain a phenomenon exhibited by a system and are usually expressed as a mathematical relation.

Such rules are observed by repeated experimentation.

Differential equations meet the conditions for expressing physical laws

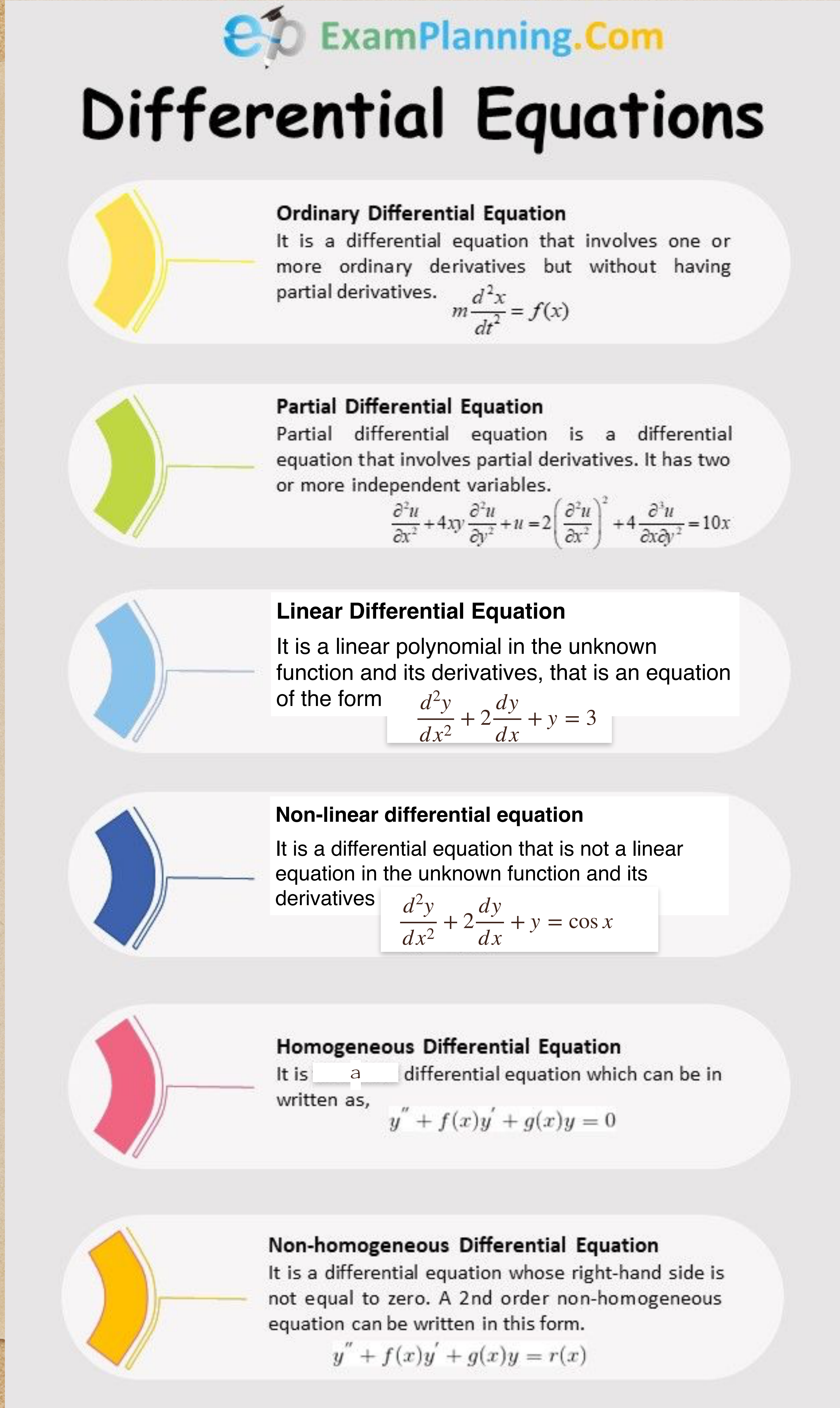
* From Lecture notes by Shabnam Siddiqui

Types of differential equations

Differential equations can be divided into several types. Common variants are :

- Ordinary,
- Partial,
- Linear,
- Nonlinear,
- Homogeneous,
- Heterogeneous.

This list is far from exhaustive.



The N-body problem

The classical astrophysical N-body problem consists of each member of an aggregate of N ($i=1,\ldots,N$) point masses, having masses m_i, experiencing an acceleration from the gravitational attractions of all the other bodies.

$$\frac{d^2\mathbf{r}_i}{dt^2} = -\sum_{j=1;j\neq i}^{N} \frac{Gm_j(\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

The description of the problem is completed by specifying the initial positions (r_i at $t = 0$) and velocities (v_i at $t=0$) for the N particles.

The globular cluster M80 (NGC 6093). Image credit: NASA, The Hubble Heritage Team, STScI, AURA

Solutions of this problem range from the orbit of the moon to the structure of the Kirkwood gaps in the asteroid belt and countless other phenomena

This richness arises from strong nonlinearity in the equation as a slight change in initial conditions can lead to very different outcomes

The problem is solved by converting the N second order differential equations into a set of 2N coupled first-order equations

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i$$

$$\frac{d\mathbf{v}_i}{dt} = -\sum_{j=i;j\neq i}^{N} \frac{Gm_j(\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

First order equations are easy to numerically integrate

The Andromeda Galaxy with satellite galaxies M32, (centre left above the galactic nucleus) and M110, (centre left below the galaxy)

Fundamental Frames

There are two fundamental frames for describing the physical governing equations of hydrodynamics

- the Lagrangian is a material description, typically used in the finite element methods (FEM).
- the Eulerian is a spatial description, typically used in finite difference methods (FDM).

If viscosity, heat conduction and external forces are neglected, the conservations equations in PDE form in the two methods are very different:

Conservation	Lagrangian description	Eulerian description
Mass	$\frac{D\rho}{Dt} = -\rho \frac{\partial v^\beta}{\partial x^\beta}$	$\frac{\partial \rho}{\partial t} + v^\beta \frac{\partial \rho}{\partial x^\beta} = -\rho \frac{\partial v^\beta}{\partial x^\beta}$
Momentum	$\frac{Dv^\beta}{Dt} = -\frac{1}{\rho}\frac{\partial p}{\partial x^\beta}$	$\frac{\partial v^\beta}{\partial t} + v^\alpha \frac{\partial v^\beta}{\partial v^\alpha} = -\frac{1}{\rho}\frac{\partial p}{\partial x^\beta}$
Energy	$\frac{De}{Dt} = -\frac{p}{\rho}\frac{\partial v^\beta}{\partial x^\beta}$	$\frac{\partial e}{\partial t} + v^\beta \frac{\partial e}{\partial x^\beta} = -\frac{p}{\rho}\frac{\partial v^\beta}{\partial x^\beta}$

Solved at the particle and uses a total derivative

Solved at a fixed point in space and needs an extra convective derivative

In the equations p, ρ, e, v and x are pressure, density, internal energy, velocity and position vectors respectively.

The Greek subscripts α and β are the coordinate directions (e.g. x,y,z) and summation is implied over repeated indices.

The Navier-Stokes Equations

The equations of fluid dynamics (in Langrangian form) are widely used for fluid dynamics problems (σ is the total stress tensor) to model fluid motion

$$\frac{D\mathbf{r}^\alpha}{Dt} = \mathbf{v}^\alpha$$

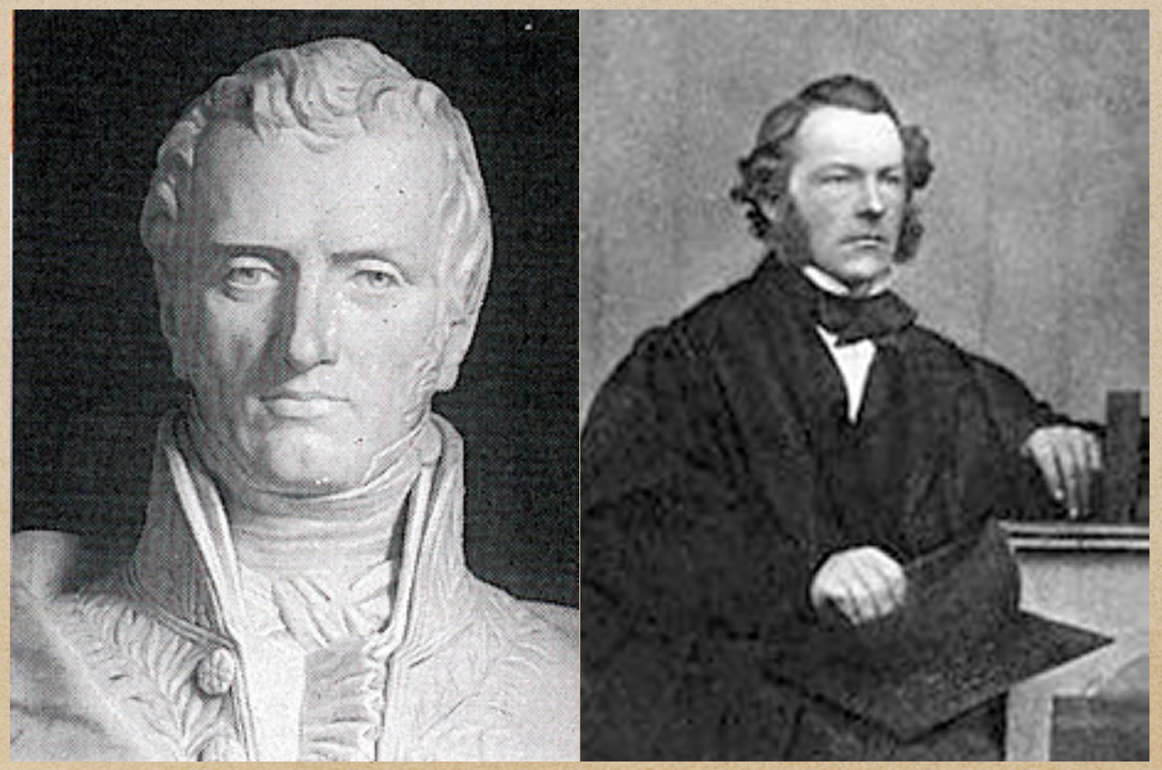
$$\frac{D\rho}{Dt} = -\rho\frac{\partial \mathbf{v}^\beta}{\partial \mathbf{r}^\beta}$$

$$\frac{D\mathbf{v}^\alpha}{Dt} = \frac{1}{\rho}\frac{\partial \sigma^{\alpha\beta}}{\partial \mathbf{r}^\beta} + F_{Gravity}$$

$$\frac{De}{Dt} = \frac{\sigma^{\alpha\beta}}{\rho}\frac{\partial \mathbf{v}^\alpha}{\partial \mathbf{r}^\beta} + E_{Heat}$$

There are many applications in Physics, Engineering, Astronomy and cosmology

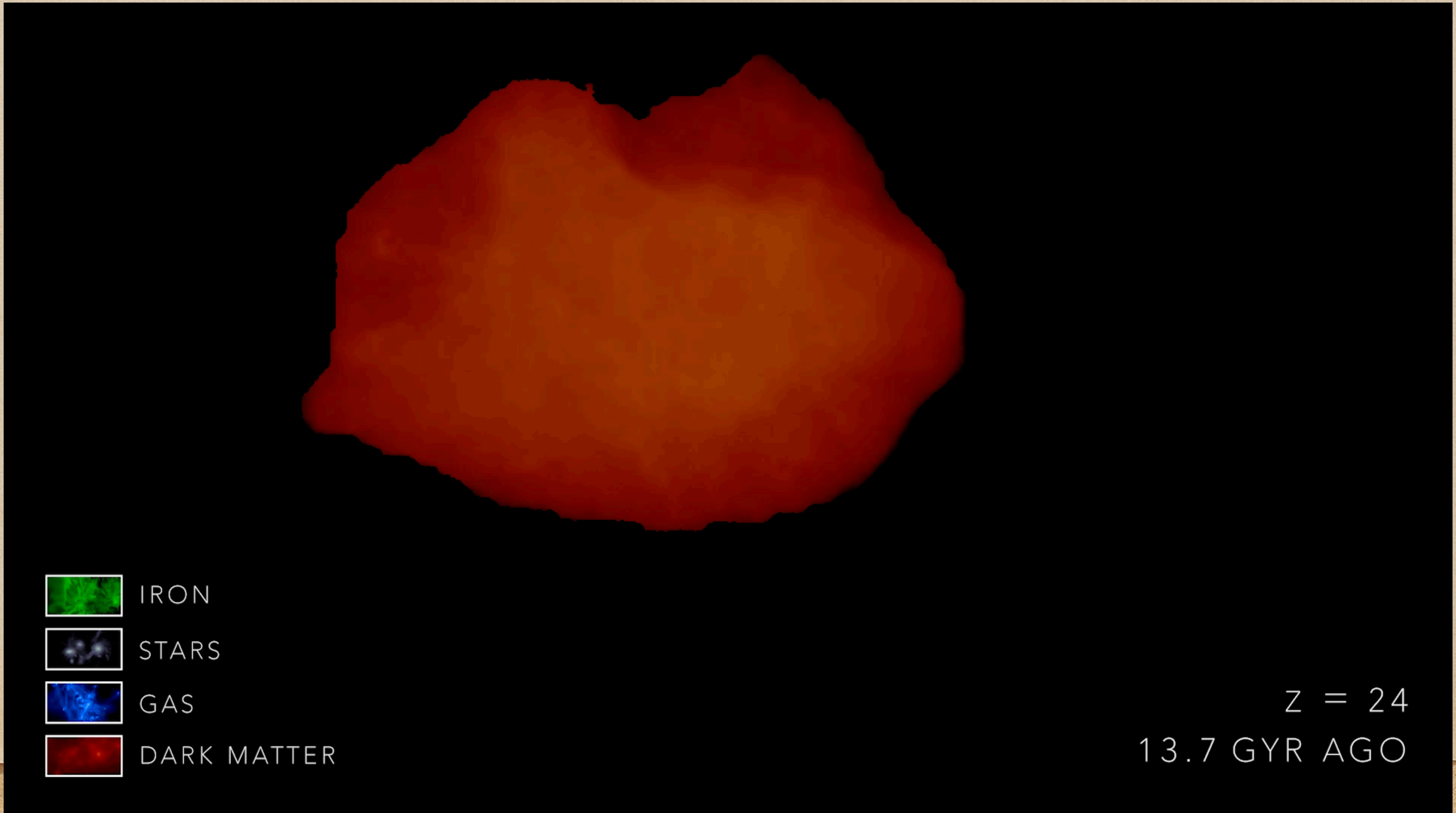
Claude-Louis Navier (10 February 1785 – 21 August 1836) was a French engineer and physicist who specialised in mechanics.



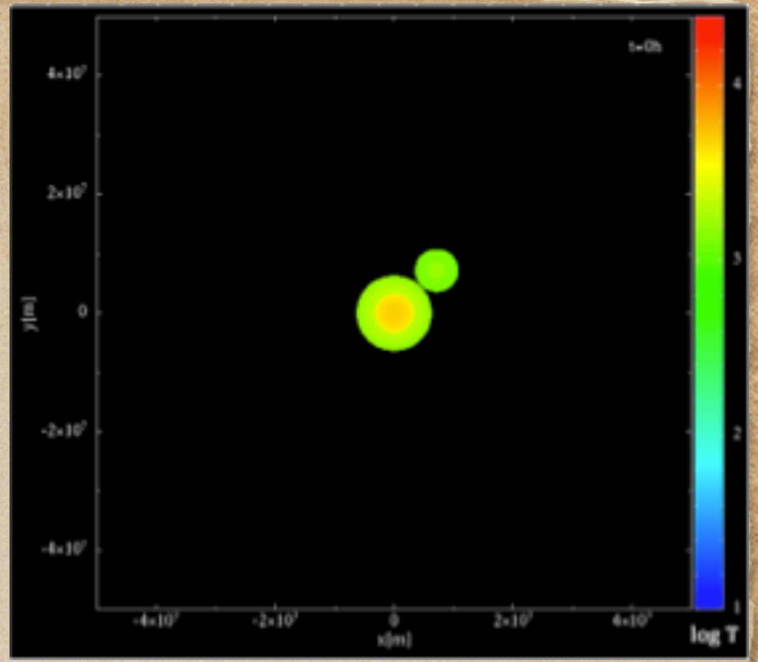
George Gabriel Stokes, (13 August 1819–1 February 1903), was a mathematician and physicist, who at Cambridge made important contributions to fluid dynamics (including the Navier–Stokes equations), optics, and mathematical physics. He was secretary, then president, of the Royal Society.

VINTERGATAN with Eulerian version of Navier Stokes

Agertz, Renaut, et al., Lund Observatory



Lunar Formation with Navier Stokes



R. Wissing and D. Hobbs: A new equation of state applied to planetary impacts. II.

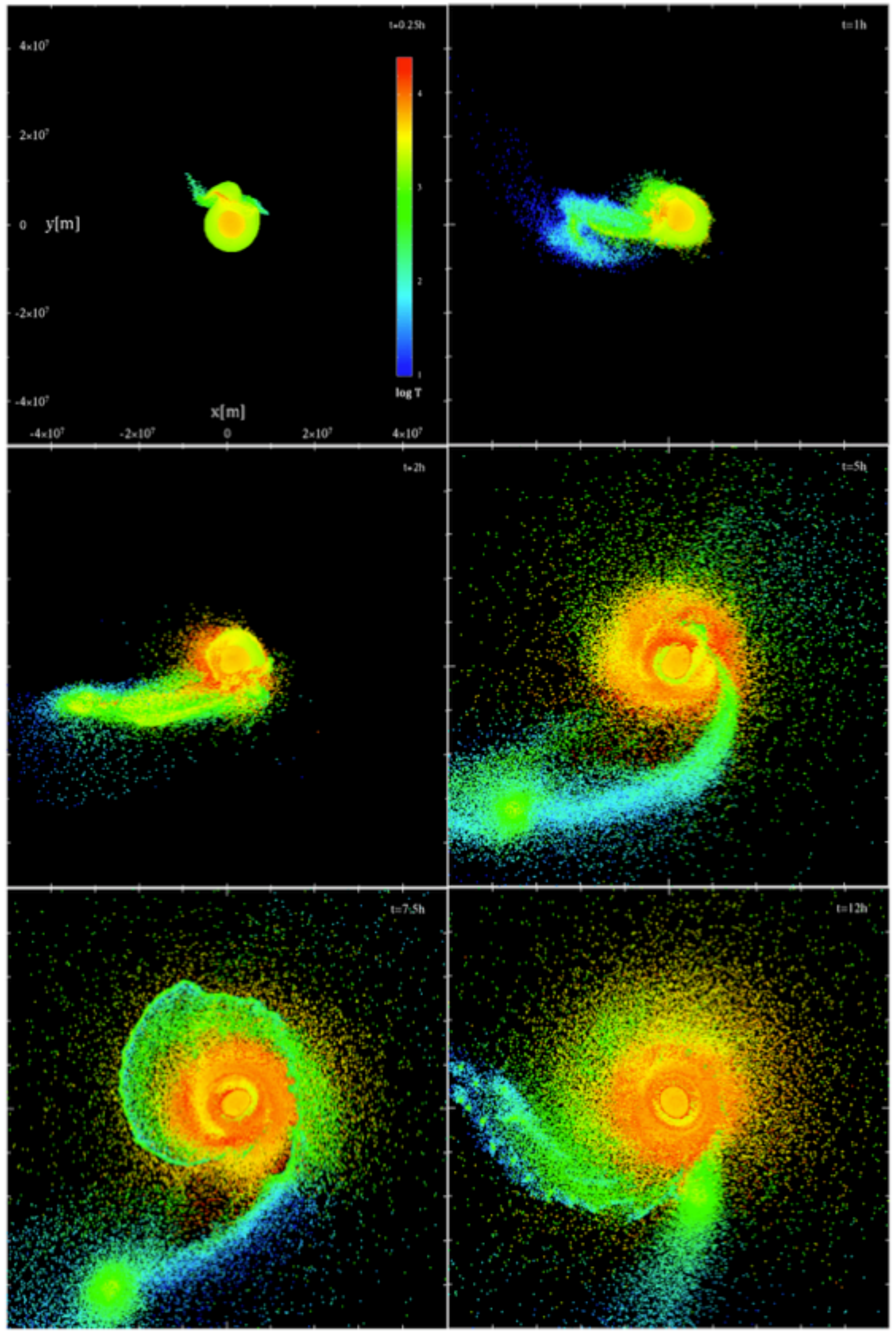


Fig. 6. Top-down view of the evolution of the collision for the $Hrc1_{\mathrm{Solid}}$ simulation. The temperature range and spatial range can be seen in the *top left figure*. The times when each of the images were captured, starting from the upper left, are $t = 0.25$, 1, 2, 5, 7.5, 12 h.

The Navier Stokes equations can be used to model any kind of fluid even the Earth-Theia collision which may have led to the formation of the moon (in this case $1.23M_{moon}$)

A&A 643, A40 (2020)

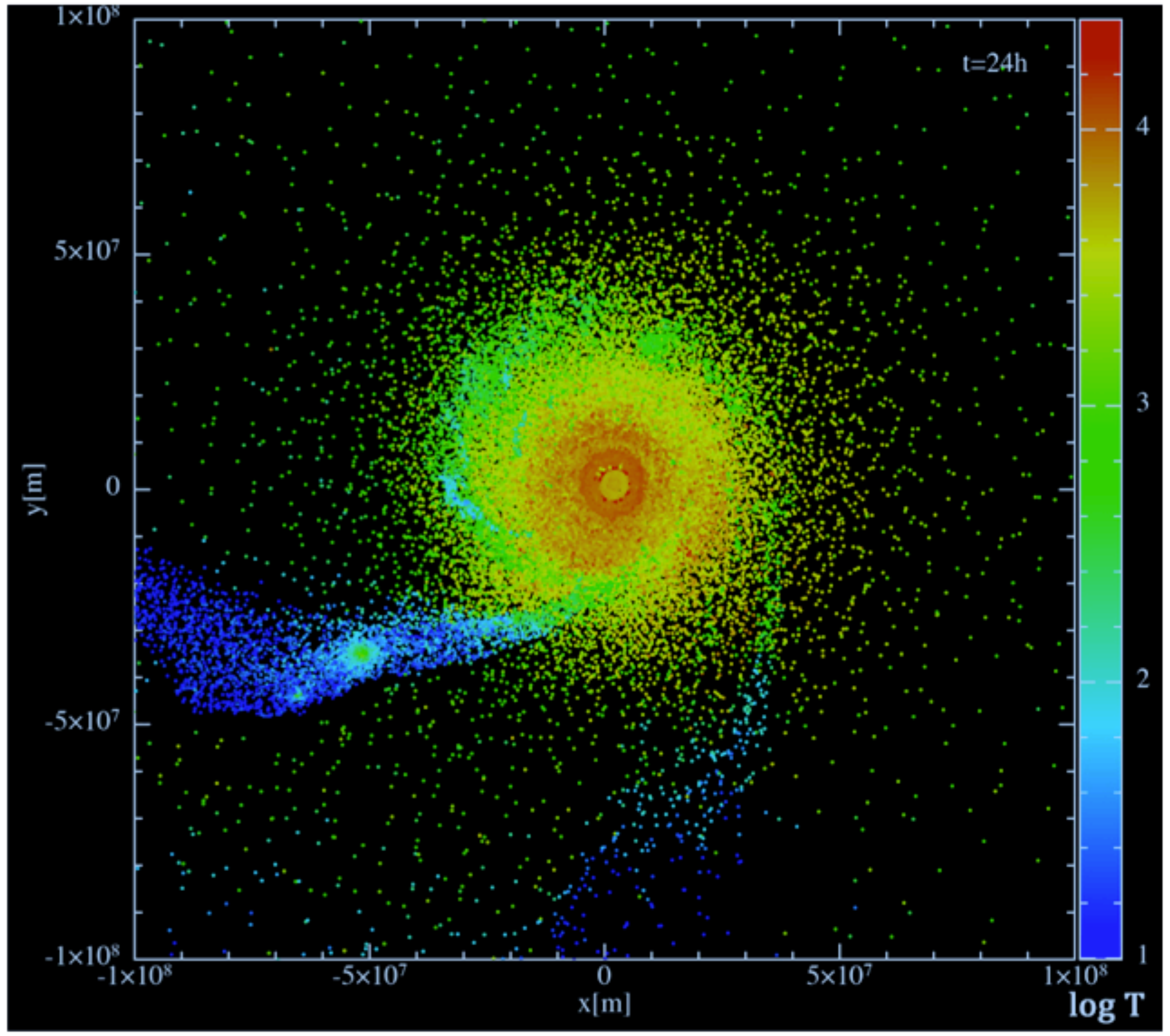


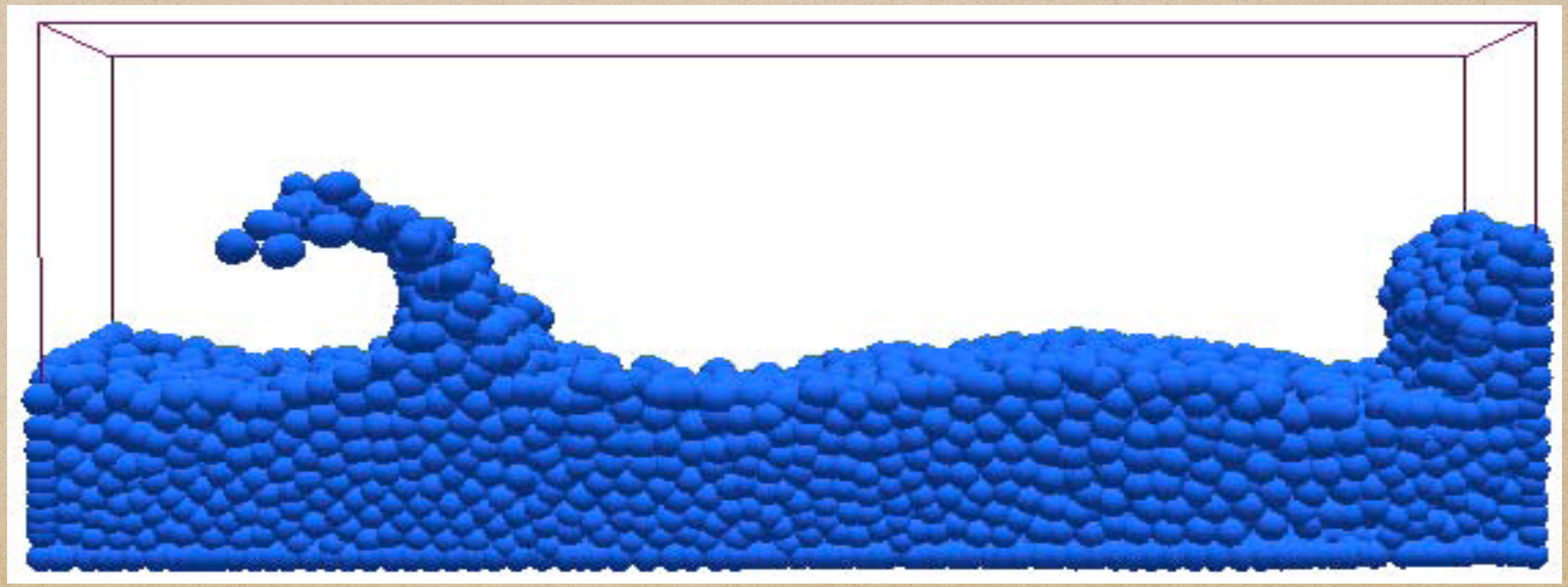
Fig. 7. State of the system after 24 h of simulation time.

Smoothed Particle Hydrodynamics (SPH)

SPH is a particle method and is inherently a Lagrangian method in which the particles represent the physical system moving in the Lagrangian frame according to internal interactions and external forces (e.g. gravity).

Advantages:

- Discretised with particles with no fixed connectivity (good for large deformations of material)
- Complex geometry is simple
- Easy to obtain large scale features by tracing the motion of the particles
- The time history of all particles is available



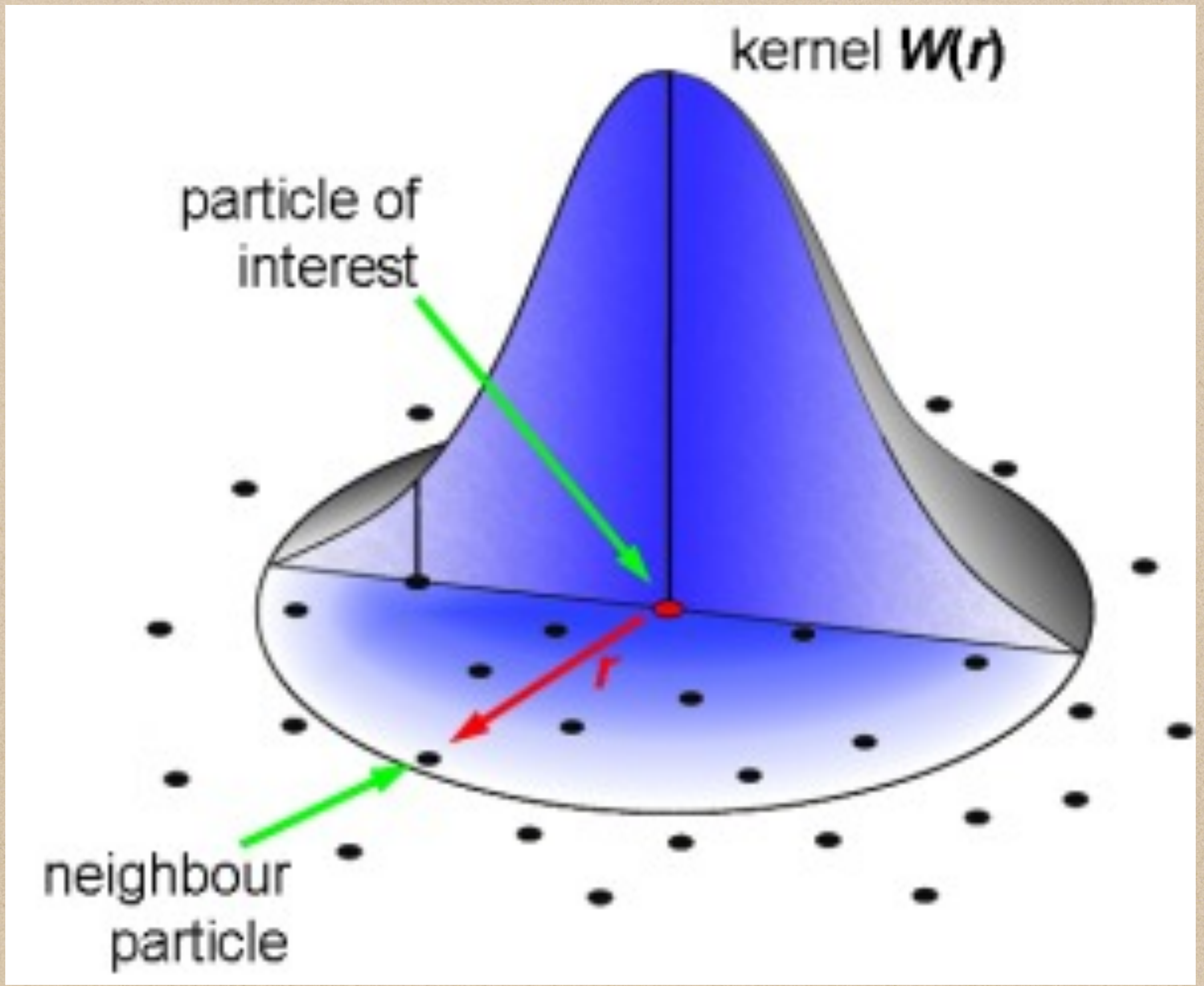
M. Kelager, Department of Computer Science, University of Copenhagen, DIKU

Solution strategy of meshfree particle methods like SPH

Approximate the functions - derivatives and integrals - using the information from neighbouring particles in an area of influence within the support domain.

E.g. the velocity v of a particle at r is:

$$\mathbf{v}(r) = \sum_{i=1}^{N} \mathbf{v}(r_i) W(r_i)$$



Mesh-free computational fluid dynamics, NUI Galway.

Where N is the number of particles, $v_i = \mathbf{v}(r_i)$ is the velocity at particle i, $W_i = W(r_i)$ is a smoothing function at the i-th particle.

Velocity, $\mathbf{v}$, is a weighted sum over neighbouring particles.

The SPH formulation

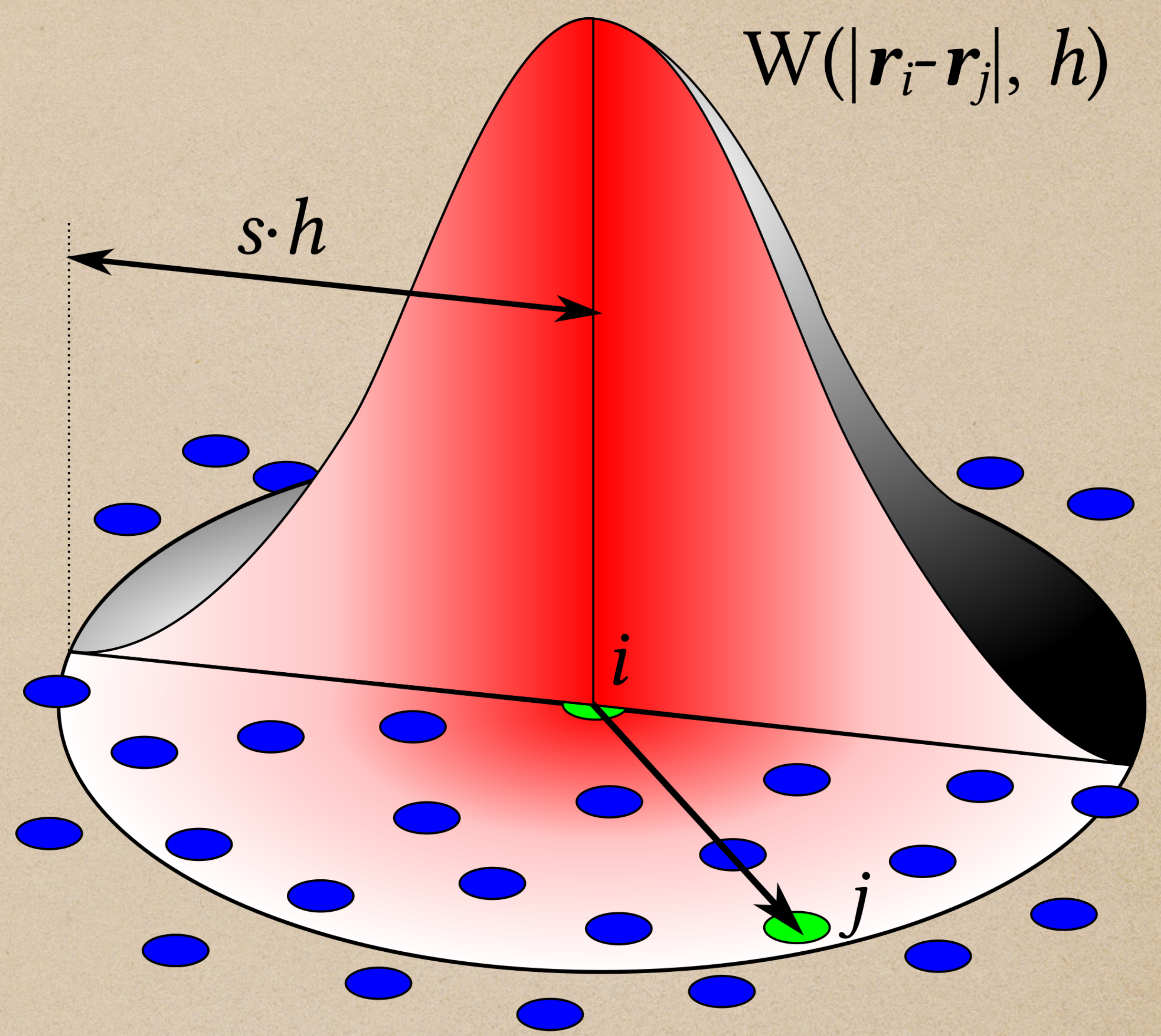
Introduction

In this lecture we introduce:

- the basic concepts of SPH
- the concepts of the support and influence domains
- Problems: how to derive SPH formulations

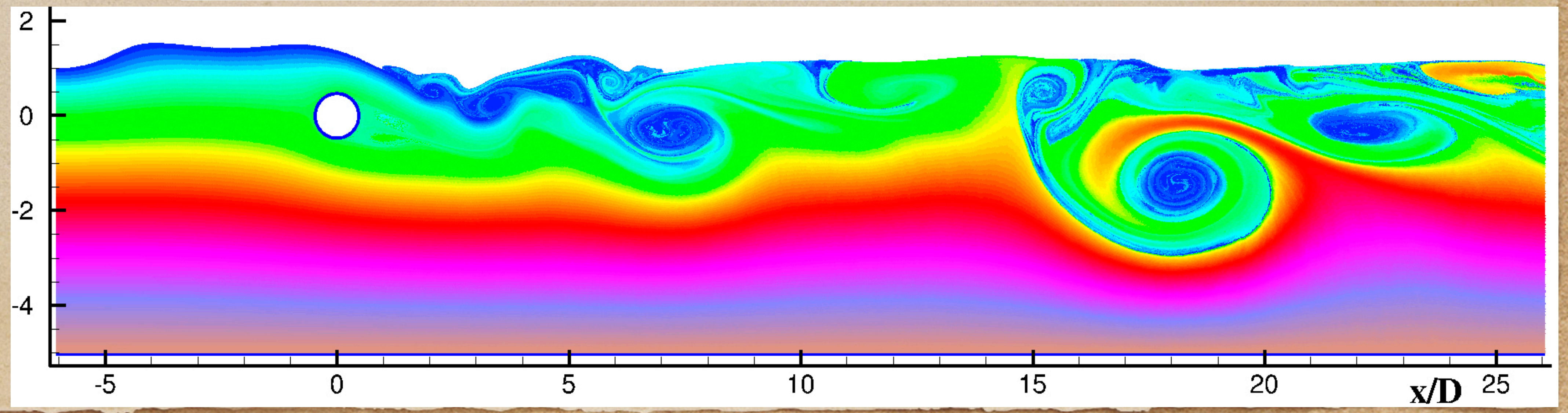
The formulation of SPH is usually divided into two main steps

- the kernel approximation (or integral representation)
- the discretised particle approximation



Schematic view of an SPH convolution (from Wikipedia)

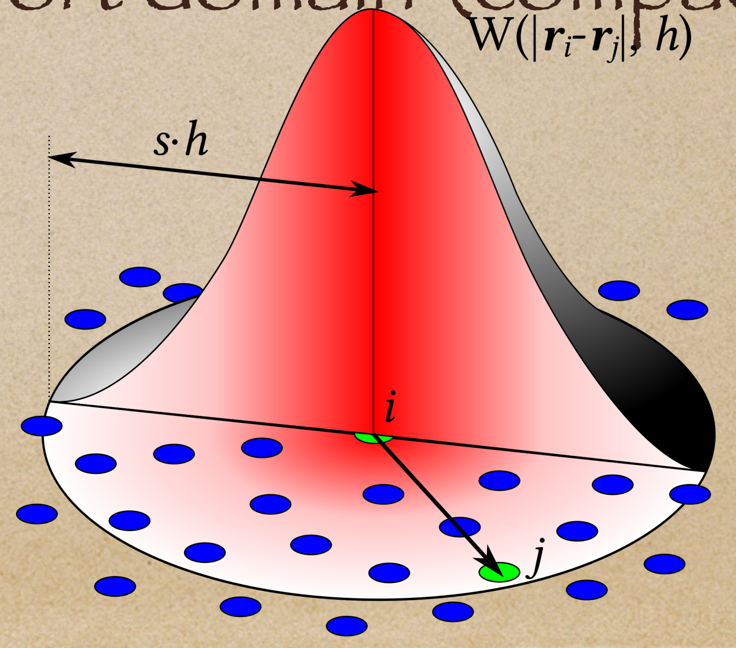
Flow around cylinder with free surface modelled with SPH (from Wikipedia)



Basic Concepts (1/2)

In the SPH method we use the following key ideas:

1. The problem domain is represented by a set of arbitrarily distributed particles and no connectivity of the particles is needed (i.e. meshfree).
2. We use an integral representation for the field functions and introduce a kernel approximation. It provides stability and has a smoothing effect.
3. The kernel approximation is then further approximated using particles. This is known as the particle approximation in SPH.
    - Done by replacing the integral representation of the function and its derivatives with summations over all corresponding values at the neighbouring particles in a local domain called the support domain (compact support).
    - Results in banded sparse matrices which can be solved efficiently



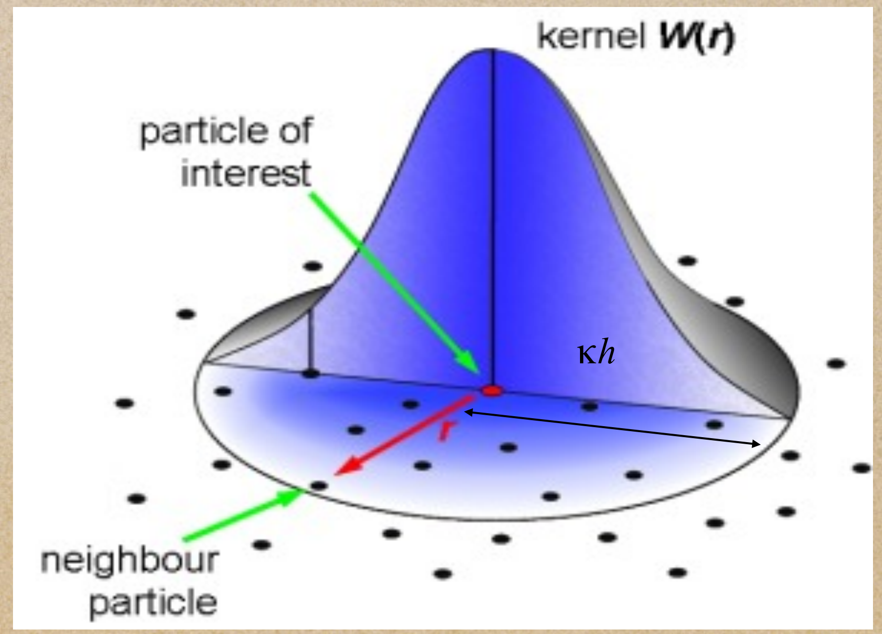
Basic Concepts (2/2)

Continued...

4. The particle approximation is performed at each time step, so particles depend on the current local distribution of particles (adaptive). Therefore, SPH naturally handles problems with large deformation.
5. The support domain must be sufficiently large and particles can be assigned mass and become physical material particles.
6. The particle approximations are performed on all field functions to produce a set of ODE's in discretised form with respect to time only (Lagrangian). Such equations are conceptually simpler than the Eulerian equivalent.
7. The ODE's are solved using an integration algorithm to achieve fast time stepping, and to obtain the time history of all the field variables for all the particles (dynamic).

So our dynamical problem is meshfree, adaptive, stable, dynamic and Lagrangian.

The detailed formulation follows!



Integral Representation of a field function (1st main step, part I)

The concept of the integral representation (or kernel approximation) of a function $f(\boldsymbol{x})$:

$$f(\boldsymbol{x}) = \int_{\Omega} f(\boldsymbol{x}')\delta(\boldsymbol{x}-\boldsymbol{x}')d\boldsymbol{x}'$$

where f is a function of the position vector $\boldsymbol{x}$, and $\delta(\boldsymbol{x} - \boldsymbol{x}')$ is the Dirac delta function

$$\delta(\mathbf{x}-\mathbf{x}') = \begin{cases} \infty & \mathbf{x}=\mathbf{x}' \\ 0 & \mathbf{x}\neq\mathbf{x}' \end{cases} \qquad \int_{-\infty}^{\infty} \delta(x)\, dx = 1.$$

and Ω is the volume of the integral that contains $\boldsymbol{x}$. This is exact as long as $f(\boldsymbol{x})$ is defined and continuous in Ω. Replace the Dirac delta by a smoothing function $W(\boldsymbol{x} - \boldsymbol{x}',h)$:

$$f(\boldsymbol{x}) \doteq \int_{\Omega} f(\boldsymbol{x}')W(\boldsymbol{x}-\boldsymbol{x}',h)d\boldsymbol{x}' \qquad \textbf{(kernel approximation)}$$

where W is the smoothing kernel function or smoothing function or kernel for short.

The smoothing length, h, defines the influence area of W.

Note, the relationship is approximate, that’s why we say kernel approximation.

This approximation is usually written with angle brackets as

$$< f(\boldsymbol{x}) >= \int_{\Omega} f(\boldsymbol{x}')W(\boldsymbol{x}-\boldsymbol{x}',h)d\boldsymbol{x}' \tag{1}$$

The smoothing function is chosen to be an even function and it satisfies a number of conditions. Firstly, the normalisation (or unity) condition:

$$\int_{\Omega} W(\boldsymbol{x}-\boldsymbol{x}',h)d\boldsymbol{x}' = 1$$

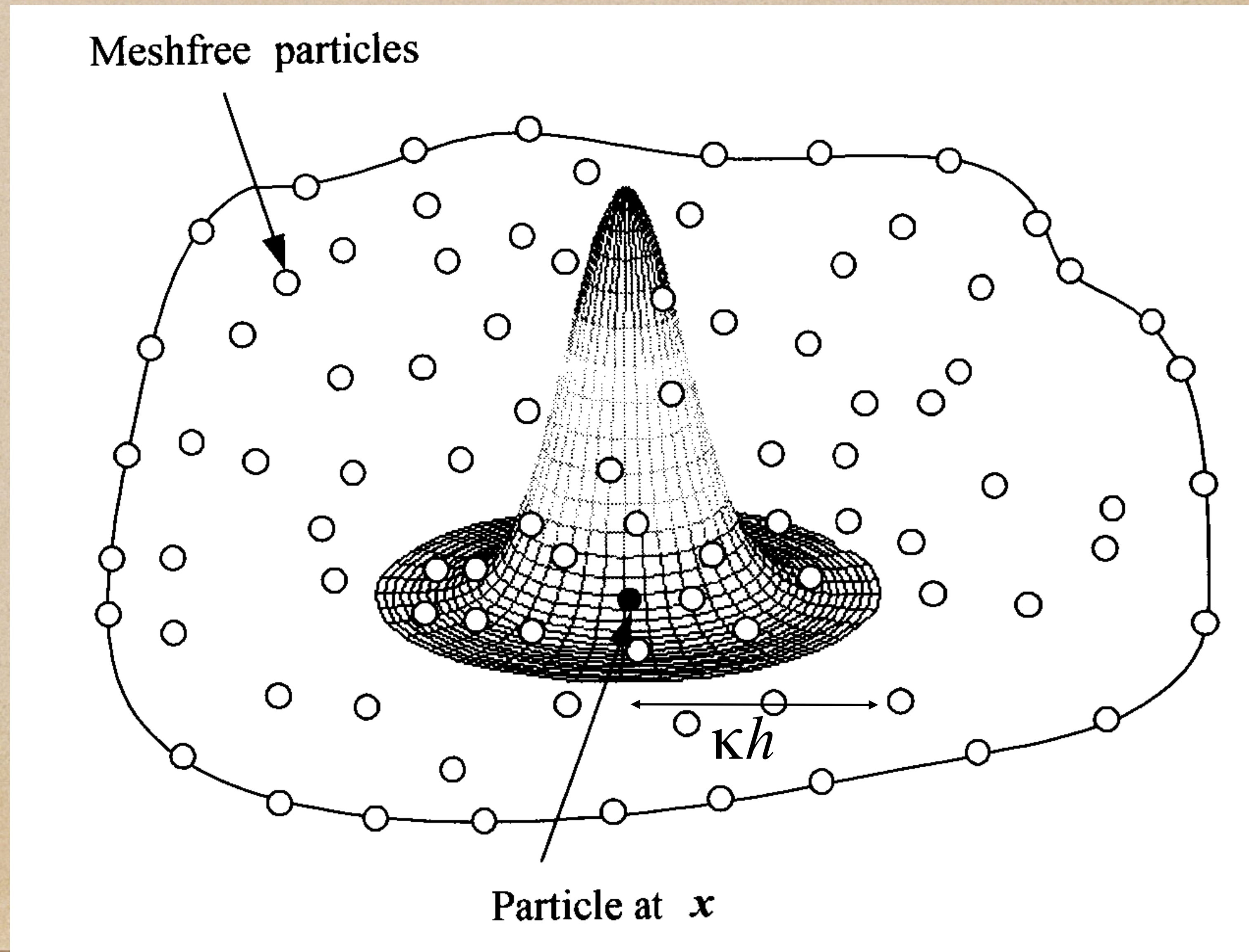
Secondly, the Delta function is recovered as the smoothing length approaches zero

$$\lim_{h\to 0} W(\boldsymbol{x}-\boldsymbol{x}',h) = \delta(\boldsymbol{x}-\boldsymbol{x}')$$

The third condition is the compact condition

$$W(\boldsymbol{x}-\boldsymbol{x}',h) = 0 \quad \text{when} \quad |\boldsymbol{x}-\boldsymbol{x}'| > \kappa h$$

Where κ is a constant and defines the non-zero area of the smoothing function called the support domain. This condition localises the support domain of the smoothing function. <u>The kernel approximation is of 2nd order accuracy if *W* is an even function.</u>



We can show this by expanding *f*(***x***') around ***x*** using a Taylor series. From:

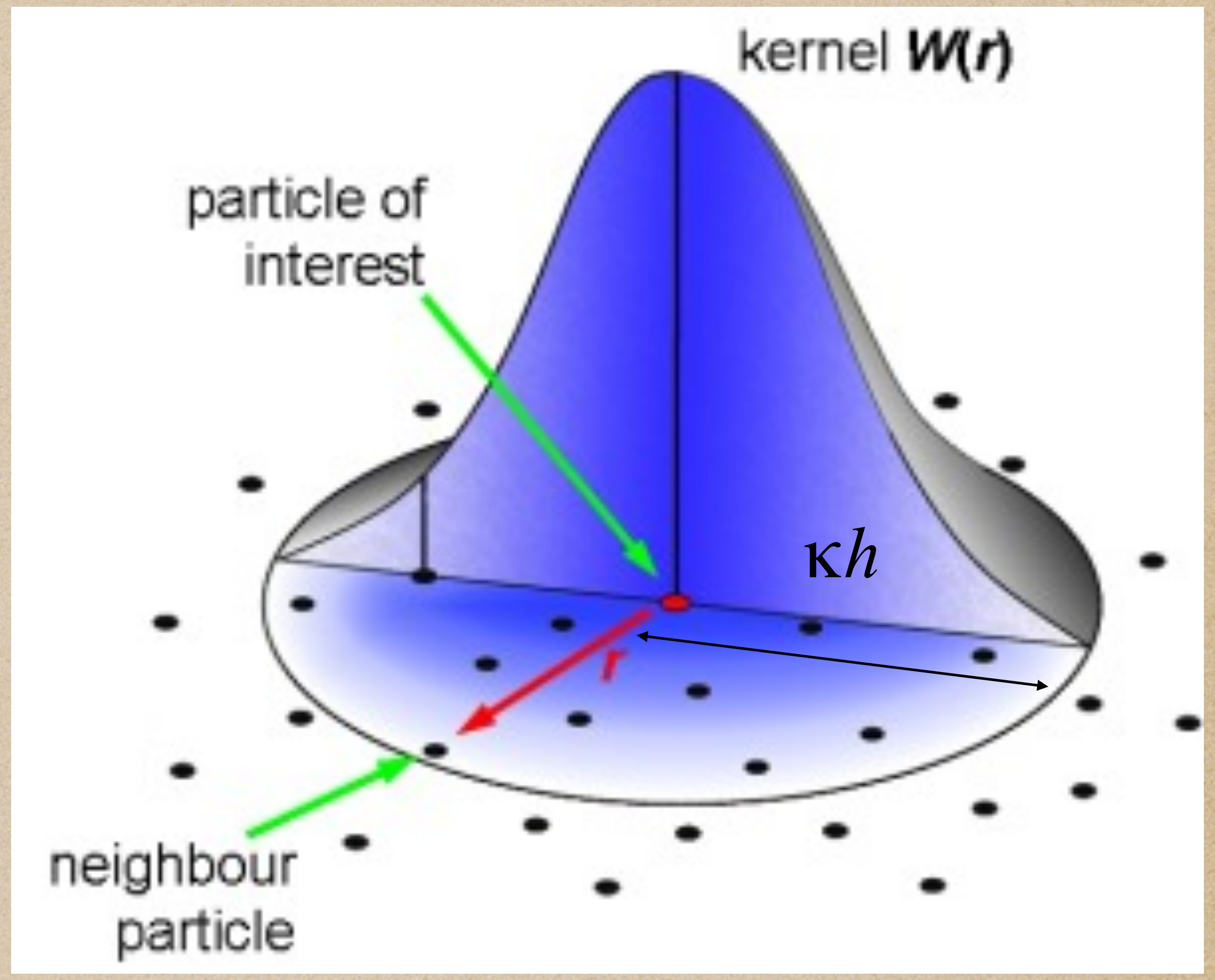
$$< f(\boldsymbol{x}) >= \int_{\Omega} f(\boldsymbol{x}')W(\boldsymbol{x}-\boldsymbol{x}',h)d\boldsymbol{x}'$$

$$< f(\boldsymbol{x}) >= \int_{\Omega} [f(\boldsymbol{x}) + f'(\boldsymbol{x})(\boldsymbol{x}'-\boldsymbol{x}) + r((\boldsymbol{x}'-\boldsymbol{x})^2)]W(\boldsymbol{x}-\boldsymbol{x}',h)d\boldsymbol{x}'$$

$$= f(\boldsymbol{x})\int_{\Omega} W(\boldsymbol{x}-\boldsymbol{x}',h)d\boldsymbol{x}'$$

$$+ f'(\boldsymbol{x})\int_{\Omega}(\boldsymbol{x}'-\boldsymbol{x})W(\boldsymbol{x}-\boldsymbol{x}',h)d\boldsymbol{x}' + r(h^2)$$

$$r((\mathbf{x}'-\mathbf{x})^2)$$



Mesh-free computational fluid dynamics, NUI Galway.

where r are the higher order residuals. If W is an even function

$$\int_{\Omega}(\boldsymbol{x}'-\boldsymbol{x})W(\boldsymbol{x}-\boldsymbol{x}',h)d\boldsymbol{x}' = 0$$

so

$$< f(\boldsymbol{x}) >= f(\boldsymbol{x}) + r((\mathbf{x}'-\mathbf{x})^2)$$

We neglect the residuals r which are of second order. If we had not used an even function for W then the error in the approximation could be larger.

Integral Representation of the divergence of a field function (1st main step, part II)

The approximation for the spatial divergence $\nabla \cdot f(\boldsymbol{x})$ is obtained by simply substituting $f(\boldsymbol{x})$ with $\nabla \cdot f(\boldsymbol{x})$ in equation (1).

$$< \nabla \cdot f(\boldsymbol{x}) >= \int_{\Omega} [\nabla \cdot f(\boldsymbol{x}')] W(\boldsymbol{x}-\boldsymbol{x}', h) d\boldsymbol{x}'$$

Where the divergence in the integral is on the primed coordinate

Using the product rule $\nabla \cdot [AB] = \nabla \cdot AB + A\nabla \cdot B$

$$[\nabla \cdot f(\boldsymbol{x}')] W(\boldsymbol{x}-\boldsymbol{x}', h) = \nabla \cdot [f(\boldsymbol{x}') W(\boldsymbol{x}-\boldsymbol{x}', h)] - f(\boldsymbol{x}') \cdot \nabla W(\boldsymbol{x}-\boldsymbol{x}', h)$$

Using this identity above

$$< \nabla \cdot f(\boldsymbol{x}) >= \int_{\Omega} \nabla \cdot [f(\boldsymbol{x}') W(\boldsymbol{x}-\boldsymbol{x}', h)] d\boldsymbol{x}' - \int_{\Omega} f(\boldsymbol{x}') \cdot \nabla W(\boldsymbol{x}-\boldsymbol{x}', h) d\boldsymbol{x}'$$

The first integral on the RHS can be converted using the divergence theorem into an integral over the surface S of the domain of the integration Ω.

$$< \nabla \cdot f(\boldsymbol{x}) >= \int_{S} f(\boldsymbol{x}') W(\boldsymbol{x}-\boldsymbol{x}', h) \cdot \vec{\boldsymbol{n}} dS - \int_{\Omega} f(\boldsymbol{x}') \cdot \nabla W(\boldsymbol{x}-\boldsymbol{x}', h) d\boldsymbol{x}'$$

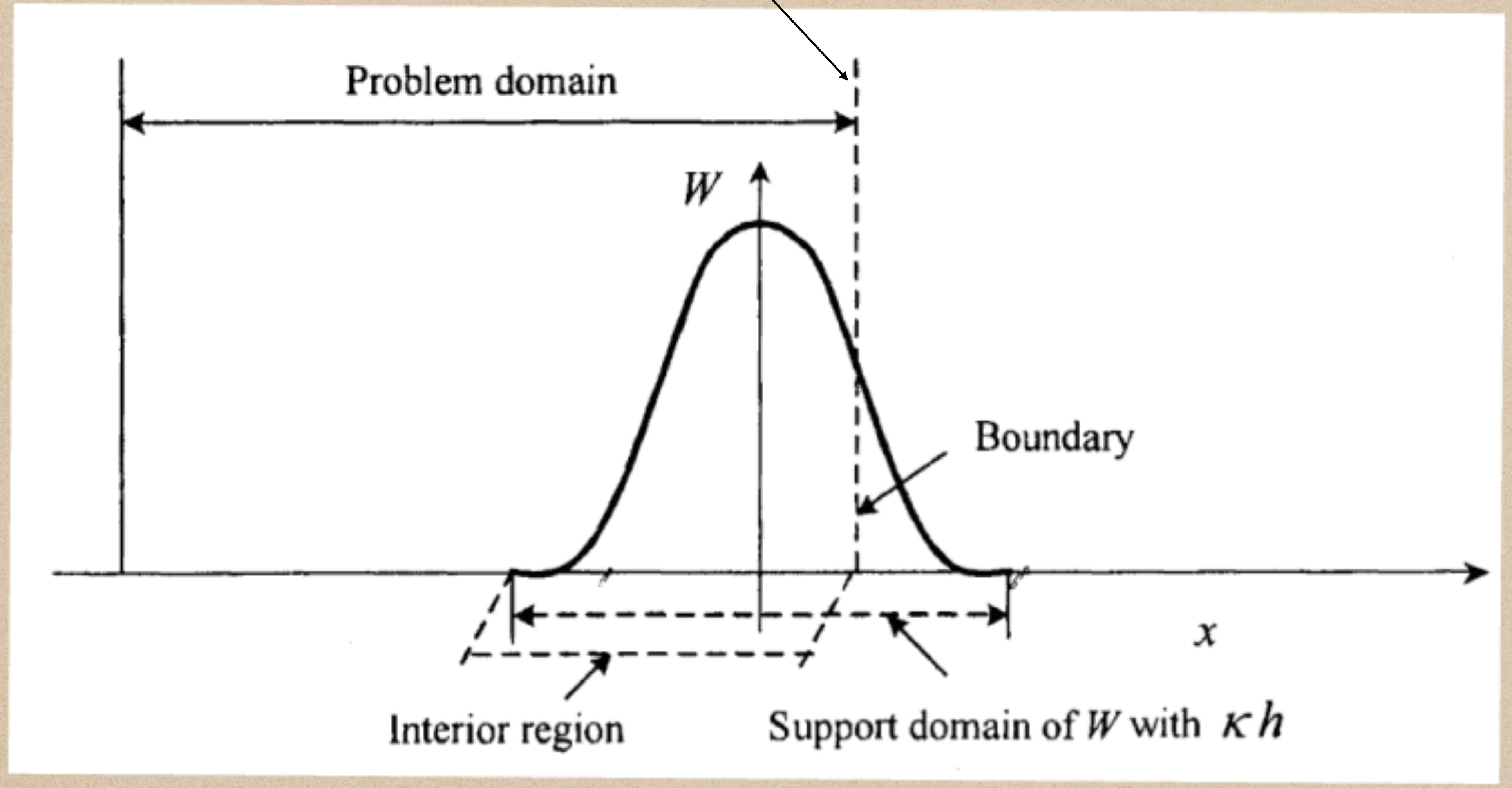
$$\iiint_V (\nabla \cdot \mathbf{F})\, dV = \iint_{\partial V} \mathbf{F} \cdot \mathbf{n}\, dS.$$

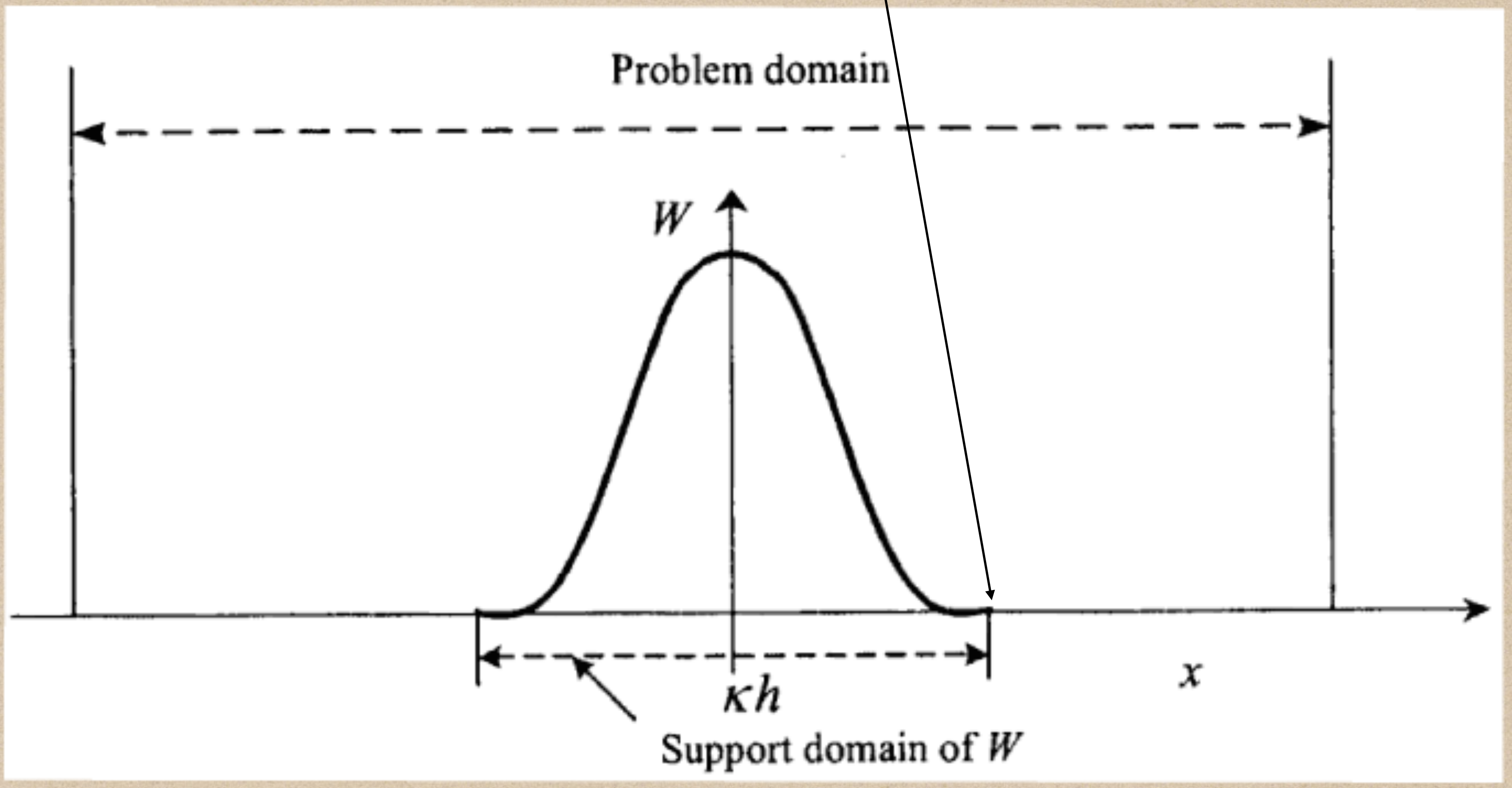
where $\boldsymbol{n}$ is the unit vector normal to the surface.

Since the smoothing function W is compact the surface integral is **just** zero and vanishes.

Note: this assumes the support domain does not overlap the problem boundary as this would be non-zero.

So for points whose support domain is inside the problem domain we have





$$< \nabla \cdot f(\boldsymbol{x}) >= -\int_{\Omega} f(\boldsymbol{x}') \cdot \nabla W(\boldsymbol{x} - \boldsymbol{x}', h) d\boldsymbol{x}' \qquad (2)$$

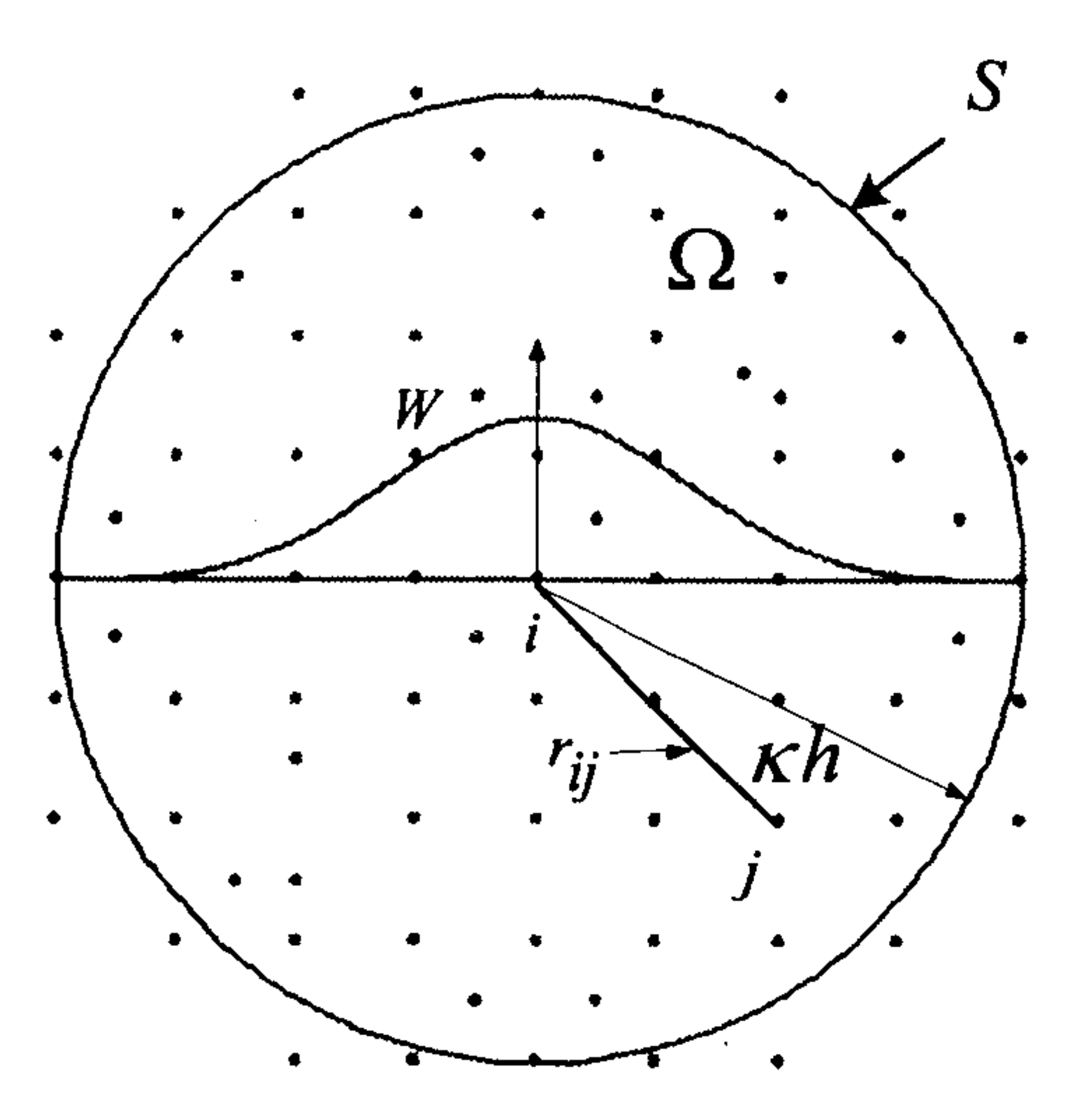
The spatial divergence of the field function can be calculated from the field function and the derivatives of the smoothing function W, rather than from the derivatives of the field function themselves.

Particle approximation (2nd main step)

Objects are represented by a finite number of particles that carry mass and occupy individual spaces. Done by applying a particle approximation, where the integrals (1) and (2) can be converted into forms with summation over all the particles in the support domain.

If the infinitesimal volume $d\boldsymbol{x}'$ at the location of particle j is replaced by the finite volume of the particle ΔV_j that is related to the mass of particles m_j by:

$$m_j = \Delta V_j \rho_j$$



Where density ρ_j is the mass per unit volume of the particle $j(=1,2,3,\ldots,N)$ in which N is the number of particles j. The SPH representation for $f(\boldsymbol{x})$ can be written in the particle approximation as

$$\begin{aligned} f(\boldsymbol{x}) &= \int_{\Omega} f(\boldsymbol{x}') W(\boldsymbol{x}-\boldsymbol{x}', h) d\boldsymbol{x}' \\ &\cong \sum_{j=1}^{N} f(\boldsymbol{x}_j) W(\boldsymbol{x}-\boldsymbol{x}_j, h) \Delta V_j \\ &= \sum_{j=1}^{N} f(\boldsymbol{x}_j) W(\boldsymbol{x}-\boldsymbol{x}_j, h) \frac{1}{\rho_j} (\rho_j \Delta V_j) \\ &= \sum_{j=1}^{N} f(\boldsymbol{x}_j) W(\boldsymbol{x}-\boldsymbol{x}_j, h) \frac{1}{\rho_j} (m_j) \end{aligned}$$

(Particle approximation)

or

$$f(\boldsymbol{x}) = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(\boldsymbol{x}_j) W(\boldsymbol{x}-\boldsymbol{x}_j, h)$$

Particle approximation for the spatial derivative:

$$<\nabla \cdot f(\boldsymbol{x})> = -\sum_{j=1}^{N} \frac{m_j}{\rho_j} f(\boldsymbol{x}_j) \cdot \nabla W(\boldsymbol{x}-\boldsymbol{x}_j, h)$$

The particle approximations are normally written as: (note that the negative sign is absorbed by $\nabla_i W_{ij}$ and is with respect to particle *i*, not *j* as derived)

$$< f(\boldsymbol{x}_i) >= \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(\boldsymbol{x}_j) \cdot W_{ij}$$

$$W_{ij} = W(\boldsymbol{x}_i - \boldsymbol{x}_j, h) = W(\left|\boldsymbol{x}_i - \boldsymbol{x}_j\right|, h)$$

The value of the function at particle *i* is approximated by using the average of the function at all particles in the support domain weighted by the smoothing function

$$< \nabla \cdot f(x_i) >= \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(x_j) \cdot \nabla_i W_{ij}$$

$$\nabla_i W_{ij} = \frac{\boldsymbol{x}_i - \boldsymbol{x}_j}{r_{ij}} \frac{\partial W_{ij}}{\partial r_{ij}} = \frac{\boldsymbol{x}_{ij}}{r_{ij}} \frac{\partial W_{ij}}{\partial r_{ij}}$$

Similarly for the divergence of the function.

The use of particle summation to approximate the integrals makes SPH simple and easy to implement.

The particle approximation introduces mass and density into the equations.

A simple way to calculate density in SPH is by summation density:

$$\rho_i = \sum_{j=1}^{N} m_j W_{ij}$$

Note the W_{ij} has units of inverse volume.

Support domain and influence domain

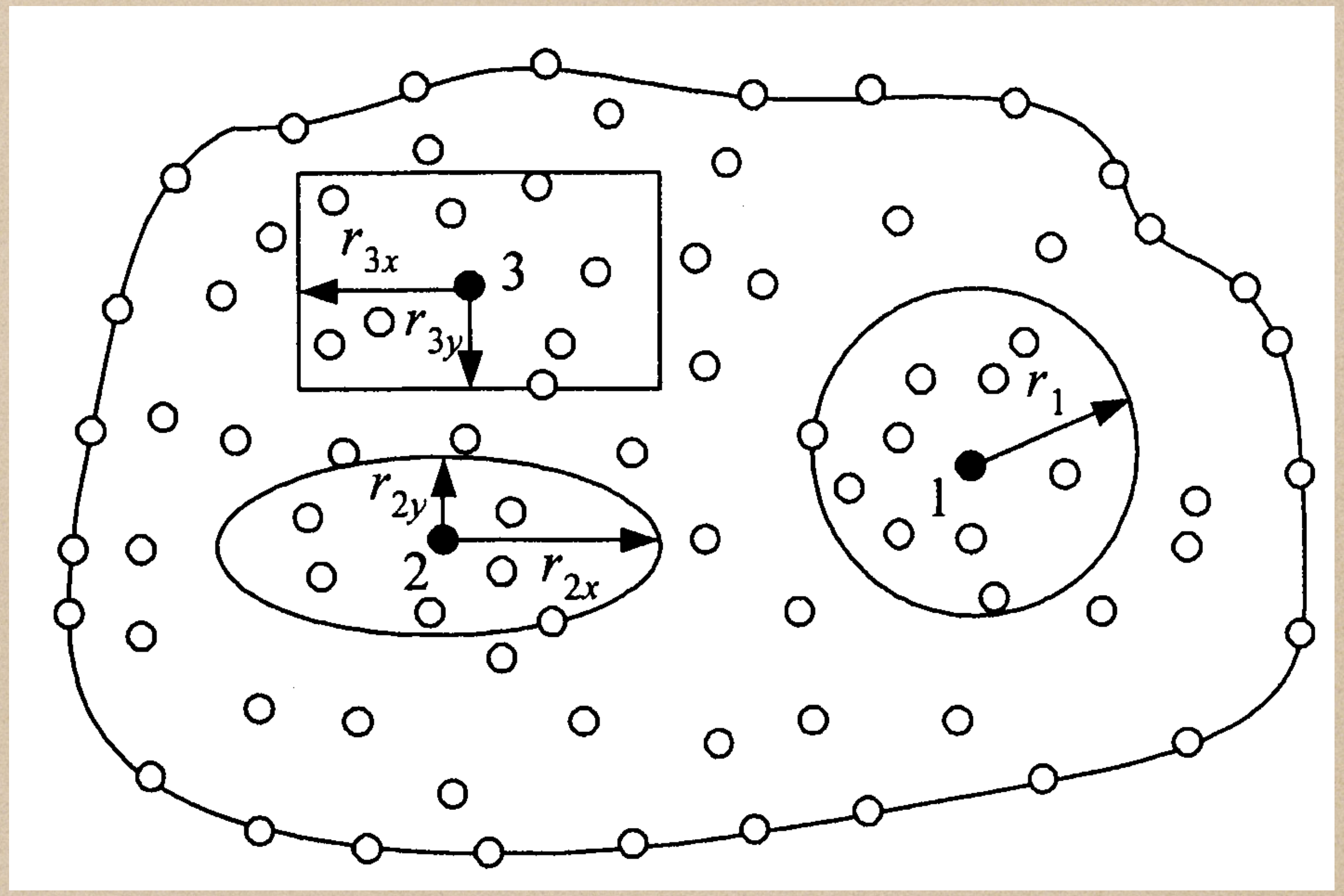
- The support domain is where all points inside this domain are used to determine the information at point $\boldsymbol{x}$.
- The influence domain is defined as the domain where a node (or particle in SPH) exerts its influence.

The influence domain is associated with a node in meshfree methods and the support domain with any field point $\boldsymbol{x}$.

As SPH is a particle method that approximates field variables only on particles (or nodes) the support and influence domains are the same.

For SPH the smoothing length h multiplied by the factor κ determines the support domain.

As can be partially seen from the figure the smoothing length can vary both spatially and temporally.



Dimensions and shapes of support domains for different points

Concluding remarks

SPH is a particle based meshfree approach.

There is no connectivity between the particles and only an initial particle distribution is needed.

The SPH approximation consists of a kernel approximation in the continuum domain and a particle approximation in the support domain at the current time step.

In the next lecture we will consider how to construct the smoothing functions introduced here.

How to derive SPH formulations

1) Using the product rule and the following vector derivative identity

$$\nabla \cdot \left(\frac{f}{\rho}\right) = \frac{\rho \nabla \cdot f - f \cdot \nabla \rho}{\rho^2}$$

show that the following two identities hold

$$\nabla \cdot f(\boldsymbol{x}) = \frac{1}{\rho}[\nabla \cdot (\rho f(\boldsymbol{x})) - f(\boldsymbol{x}) \cdot \nabla \rho]$$

$$\nabla \cdot f(\boldsymbol{x}) = \rho[\nabla \cdot (\frac{f(\boldsymbol{x})}{\rho}) + \frac{f(\boldsymbol{x})}{\rho^2} \cdot \nabla \rho]$$

2) Apply the kernel approximation

$$< \nabla \cdot f(\boldsymbol{x}) >= \int_{\Omega} [\nabla \cdot f(\boldsymbol{x}')] W(\boldsymbol{x} - \boldsymbol{x}', h) d\boldsymbol{x}'$$

using the integral representation of the divergence of a field function and apply the result of the particle approximation procedure to each divergence in the first problem to obtain the following results. Note, on the rhs objects inside the gradient terms are indexed with *j* and outside are indexed with *i*.

$$\nabla \cdot f(\boldsymbol{x}_i) = \frac{1}{\rho_i}\left[\sum_{j=1}^{N} m_j \left[f(\boldsymbol{x}_j) - f(\boldsymbol{x}_i)\right] \cdot \nabla_i W_{ij}\right]$$

$$\nabla \cdot f(\boldsymbol{x}_i) = \rho_i \left[\sum_{j=1}^{N} m_j \left[(\frac{f(\boldsymbol{x}_j)}{\rho_j^2}) + (\frac{f(\boldsymbol{x}_i)}{\rho_i^2})\right] \cdot \nabla_i W_{ij}\right]$$

The above results are rather desirable as the field function appears in the form of paired particles. These expressions are more useful in practice, produce a symmetric central force between particles, conserve linear and angular momentum and allow consistent energy equations to be constructed. This is the form used by Monaghan (1992) Annual Review of Astronomy and Astrophysics, 30:543-574.