Vortex Methods in 2D

PARTICLES : Lagrangian, Conservation and Other Laws

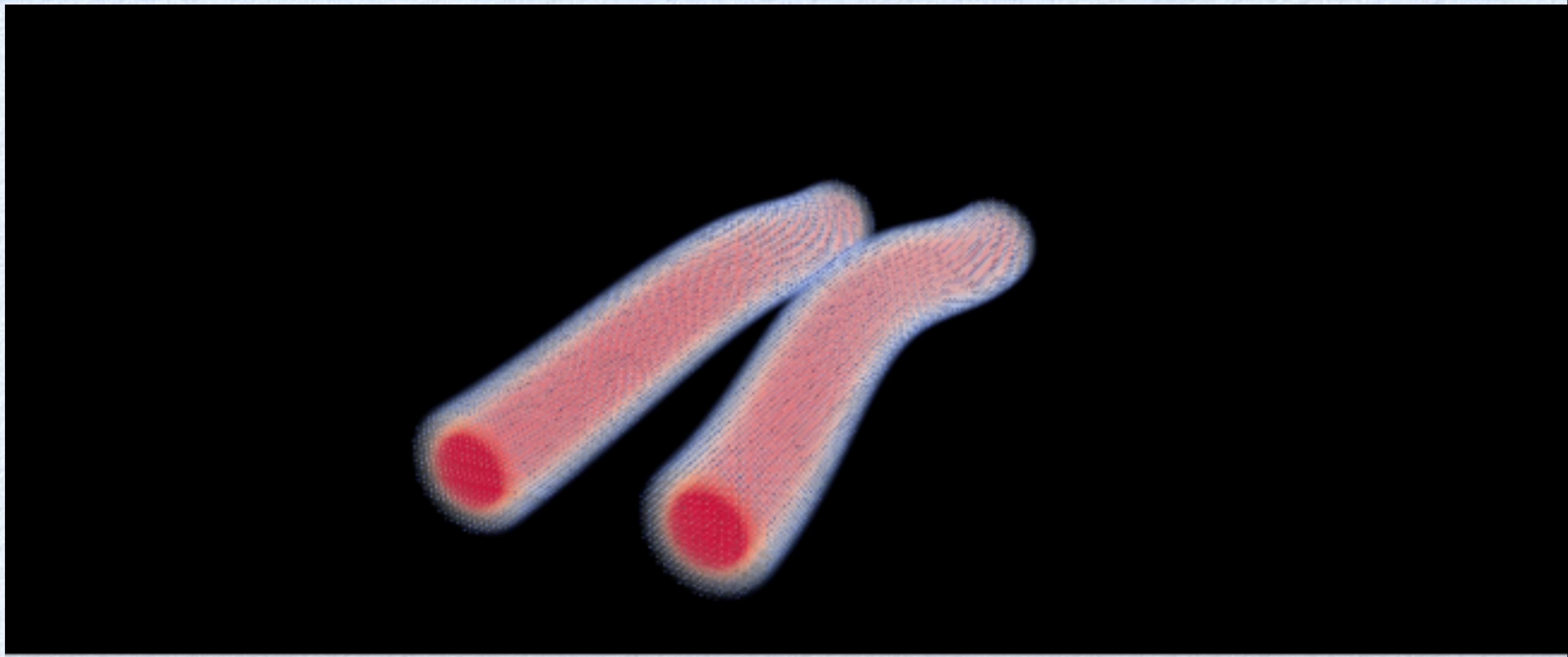
SPH, Vortex Methods

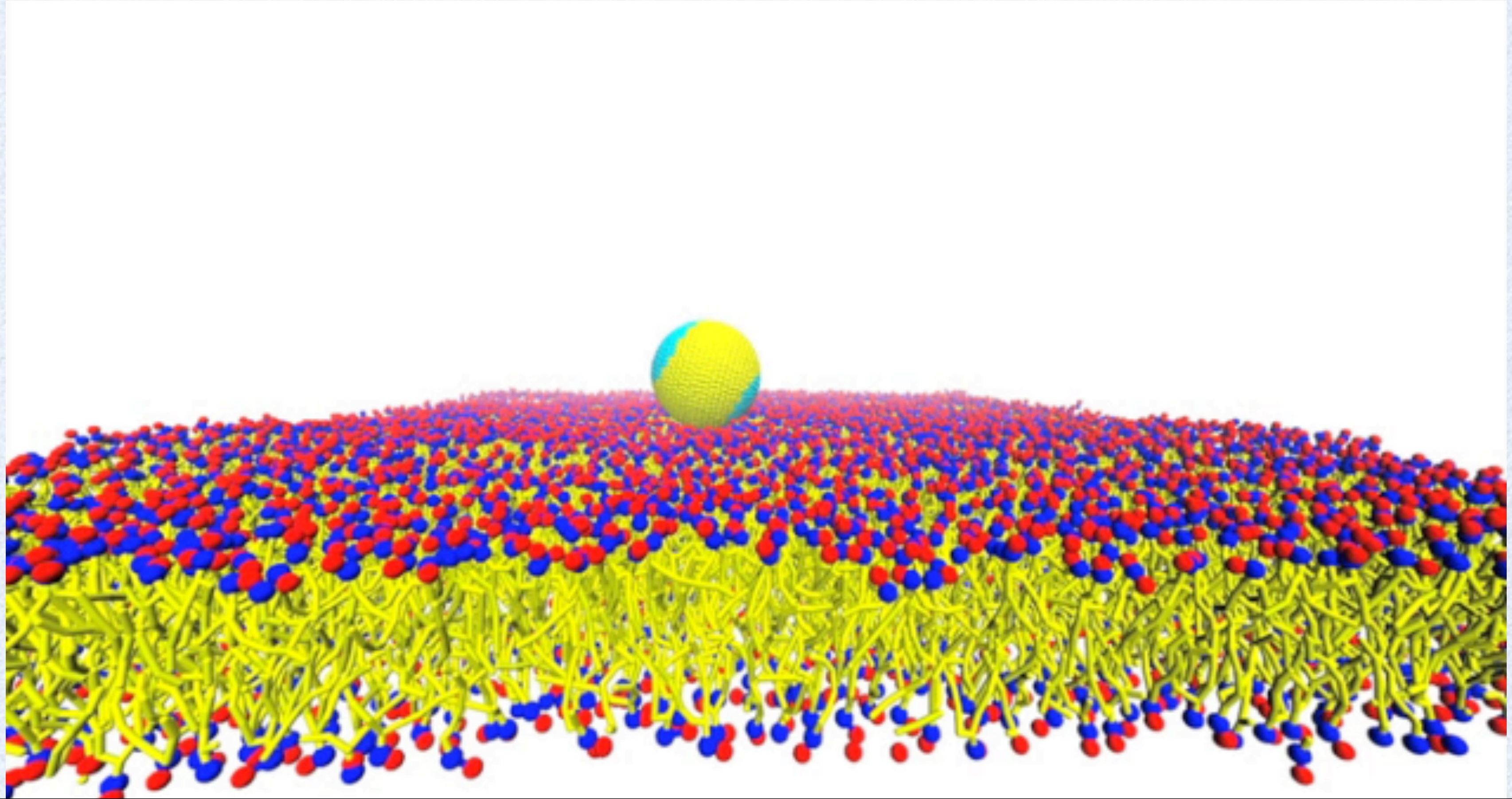
$$\rho_p \frac{D\mathbf{u_p}}{Dt} = (\nabla \cdot \sigma)_p$$

$$\frac{d\mathbf{x_p}}{dt} = \mathbf{u}_p$$

$$m \frac{d\mathbf{u_p}}{dt} = F_p$$

MD, DPD, CGMD





VORTEX METHODS (2D)

$$\omega = \nabla \times \mathbf{u}$$

Velocity-Vorticity Form of the Navier-Stokes Equations

$$\nabla \times \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \mathbf{u}\right) \quad \& \quad \nabla \cdot \mathbf{u} = \mathbf{0}$$

$$\frac{\partial \omega}{\partial t} + \mathbf{u} \cdot \nabla \omega = \nu \nabla^{\mathbf{2}} \omega \longrightarrow$$

$$\frac{D\omega}{Dt} = \nu \nabla^2 \omega$$

&

$$\frac{d\mathbf{x_p}}{dt} = \mathbf{u}_p$$

with

$$\nabla^2 \mathbf{u} = -\nabla \times \omega$$

A Fractional Step Algorithm

$$\omega(x) = \sum_{p=1}^{N} \Gamma_p(t)\, \zeta_\epsilon(x - x_p(t))$$

Advection

$$\frac{D\omega}{Dt} = 0$$

$$\nabla^2 \mathbf{u} = -\nabla \times \omega$$

$$\frac{dx_p}{dt} = u_p = \sum_{q=1}^{N} \Gamma_q K(x_p - x_q)$$

GPU

Diffusion

$$\frac{\partial \omega}{\partial t} = \nu\left(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}\right)$$

$$\Gamma_p^{n+1} = \Gamma_p^n + \frac{2\nu\delta t h^2}{\epsilon^2} \sum_{p=1}^{N} (\Gamma_p^n - \Gamma_q^n)\, \zeta_\epsilon(x_q^n - x_p^n)$$

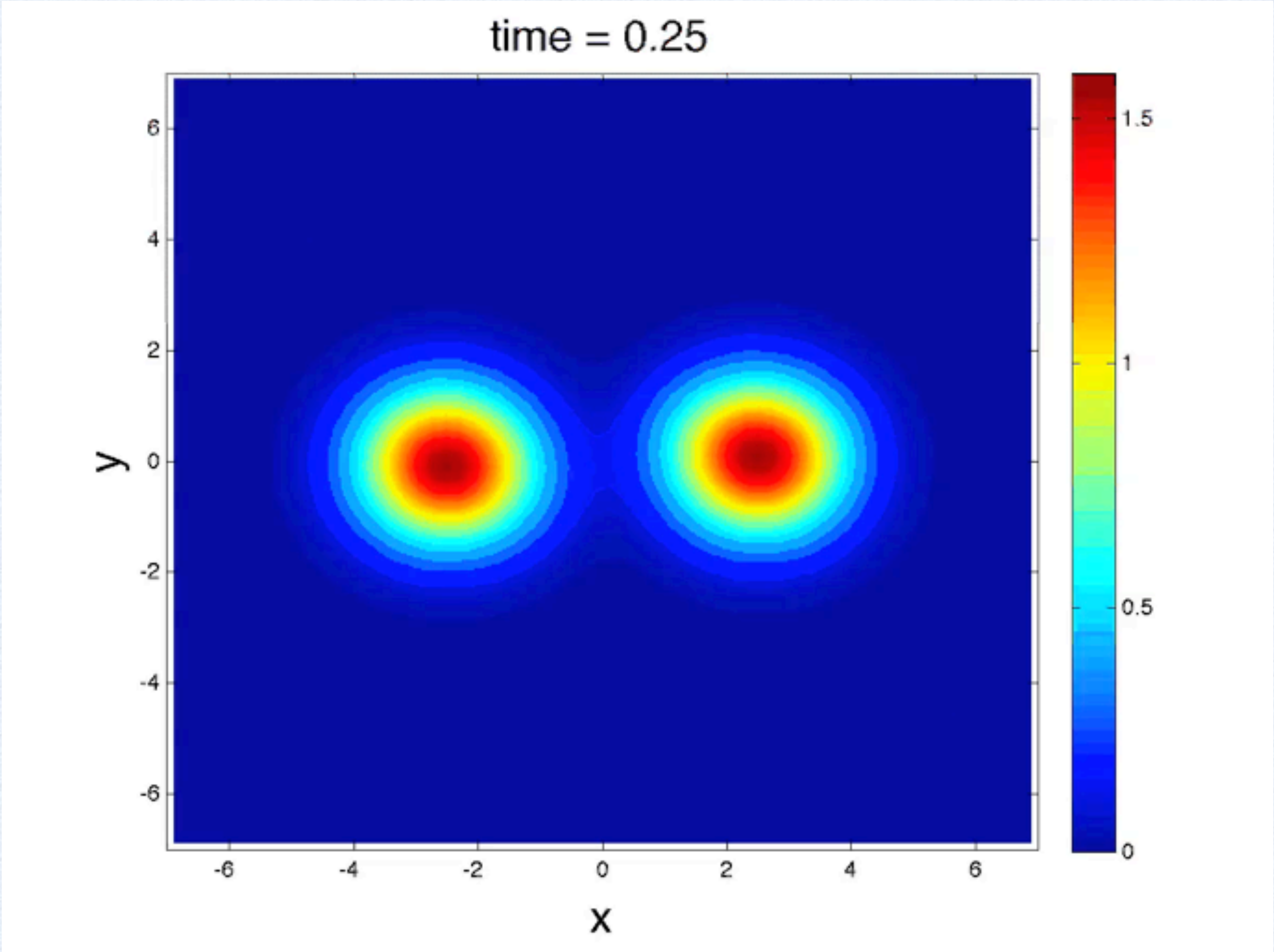
GPU

Remeshing

$$\Gamma_m = \sum_{q=1}^{M} \Gamma_q \Lambda(x_m - x_q)$$

OpenMP

Vortex Merger



ADI for Reaction-Diffusion Systems

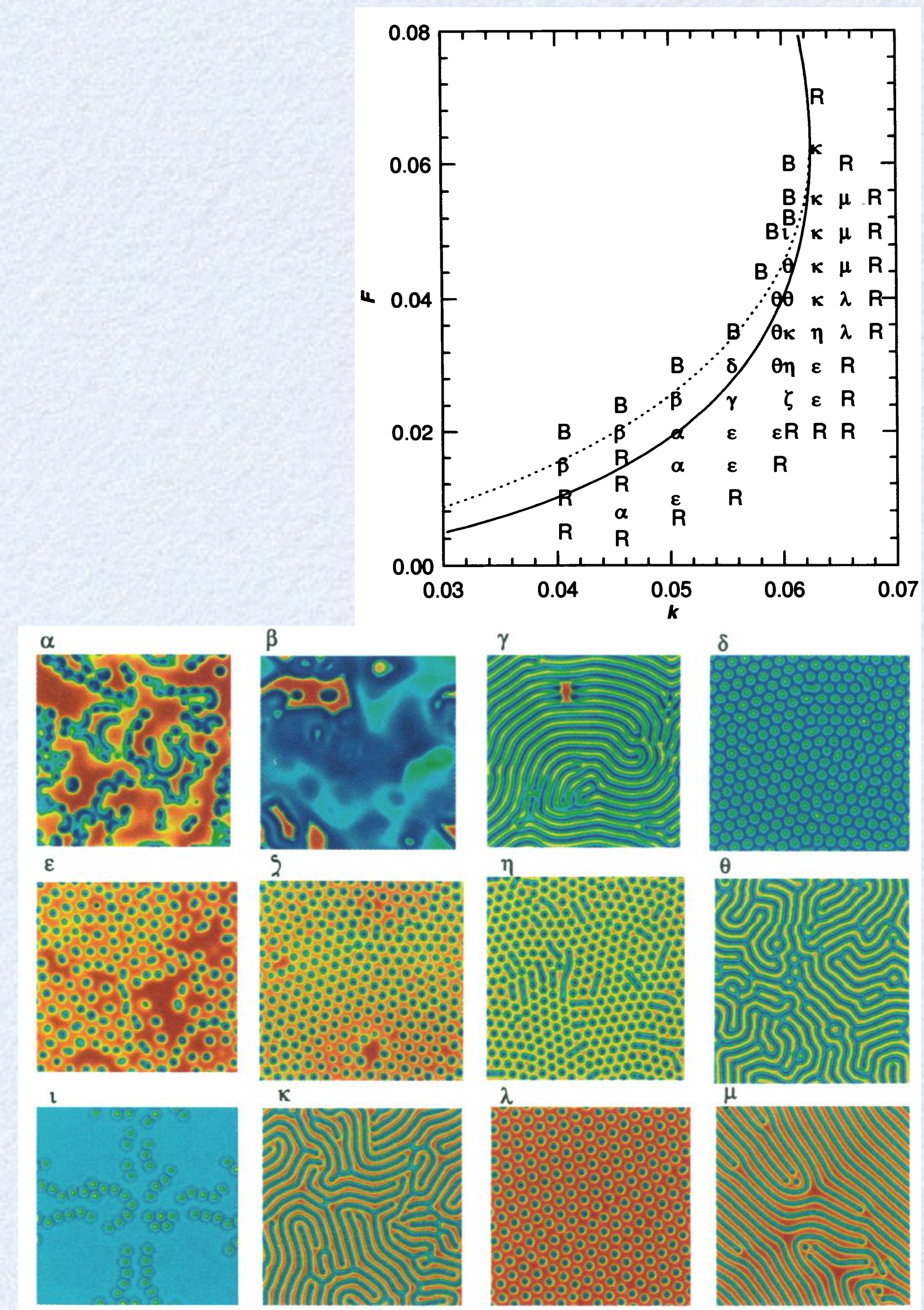
Gray-Scott reaction-diffusion

Reaction-Diffusion system (see Project 3 from HPCSE I):

$$
\begin{aligned}
\frac{\partial u}{\partial t} &= D_u \Delta u - uv^2 + F(1-u), \\
\frac{\partial v}{\partial t} &= D_v \Delta v + uv^2 - (F+k)v.
\end{aligned}
$$

u, v: chemical species

F, k: model parameters



Sample parameters:

F=0.03, k=0.062, Du=2e-5, Dv=1e-5

Alternate direction implicit

Diffusion equation $\frac{\partial \rho}{\partial t} = D_\rho \Delta \rho$ with ADI

Step 1

$$\rho_{i,j}^{n+\frac{1}{2}} = \rho_{i,j}^{n} + \frac{D\delta t}{2}\left[\frac{\partial^2 \rho_{i,j}^{n+\frac{1}{2}}}{\partial x^2} + \frac{\partial^2 \rho_{i,j}^{n}}{\partial y^2}\right]$$

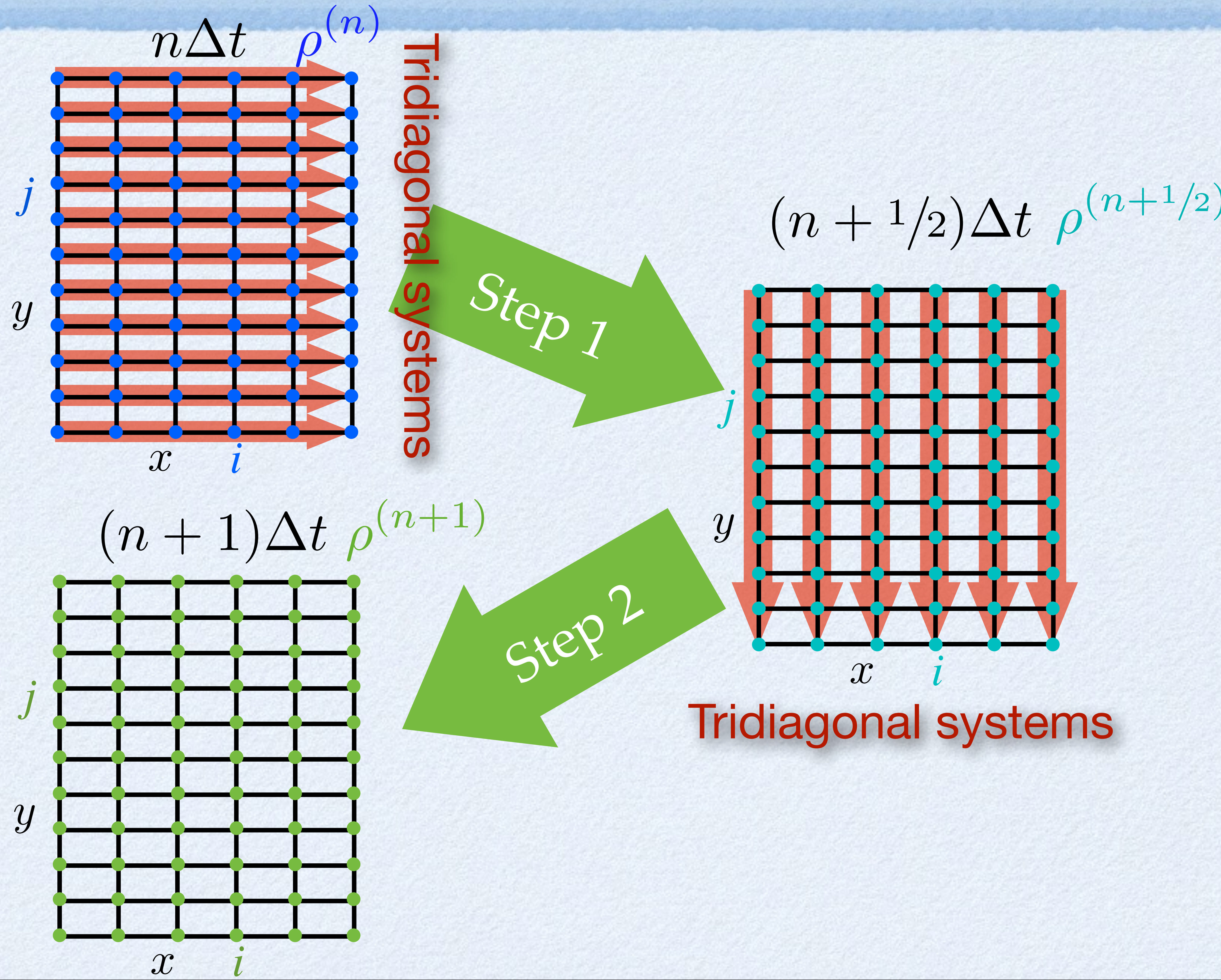
explicit

Step 2

implicit

$$\rho_{i,j}^{n+1} = \rho_{i,j}^{n+\frac{1}{2}} + \frac{D\delta t}{2}\left[\frac{\partial^2 \rho_{i,j}^{n+\frac{1}{2}}}{\partial x^2} + \frac{\partial^2 \rho_{i,j}^{n+1}}{\partial y^2}\right]$$

Alternate direction implicit



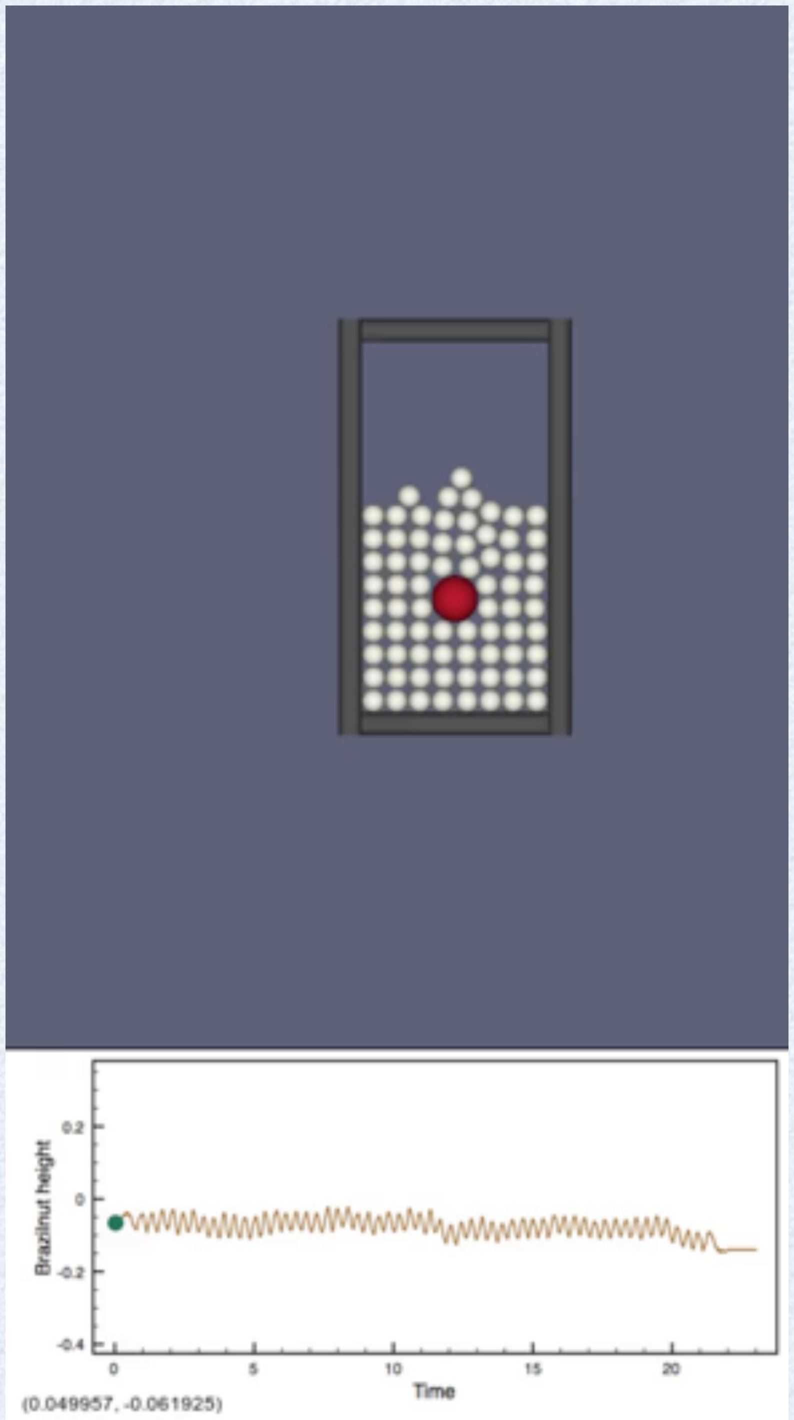
Parallel Granular Flow

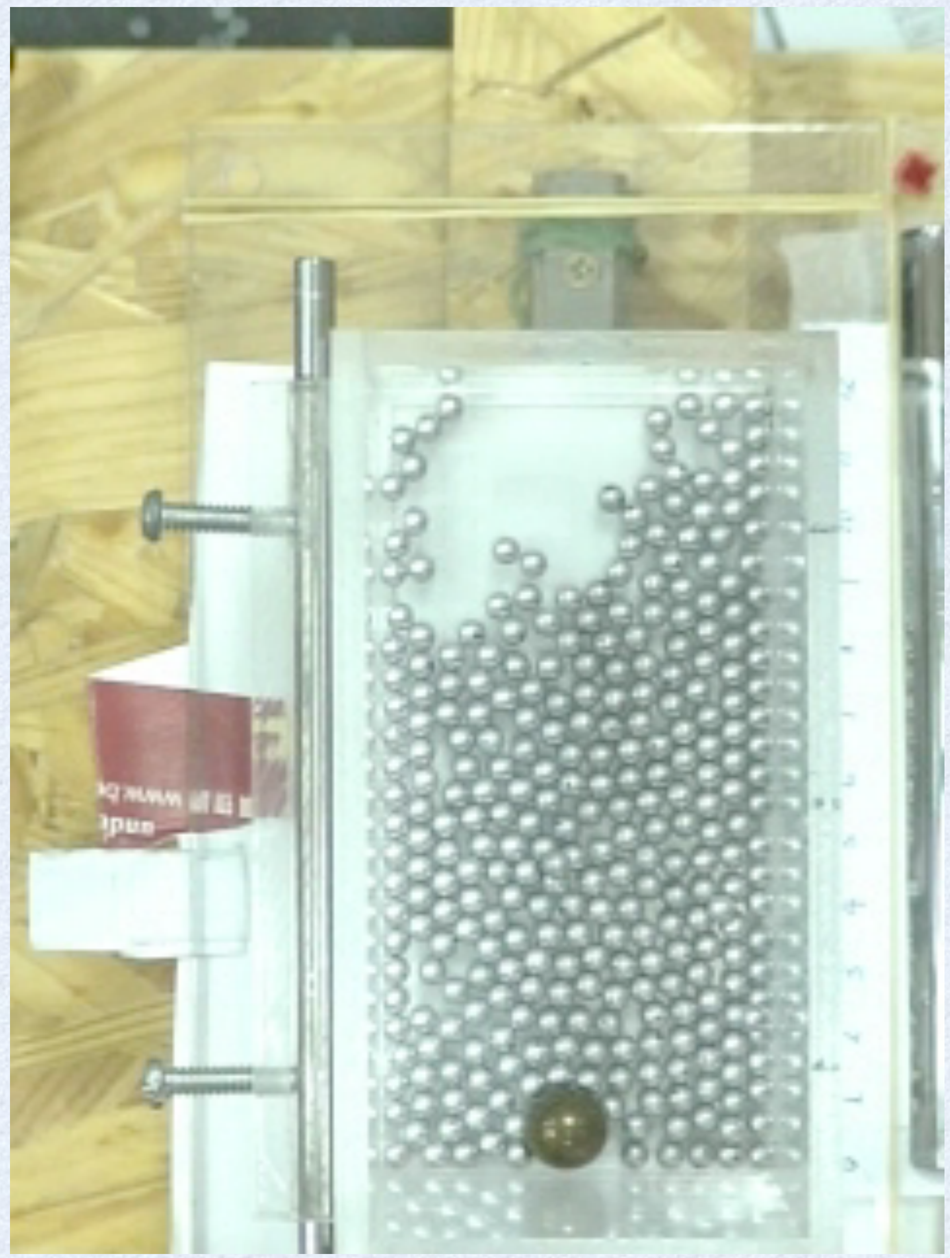
Granular flow: Discrete element method

- Discrete element method — a numerical technique for modelling particle systems by tracking each particle's movement and its interaction with its surrounding [1]

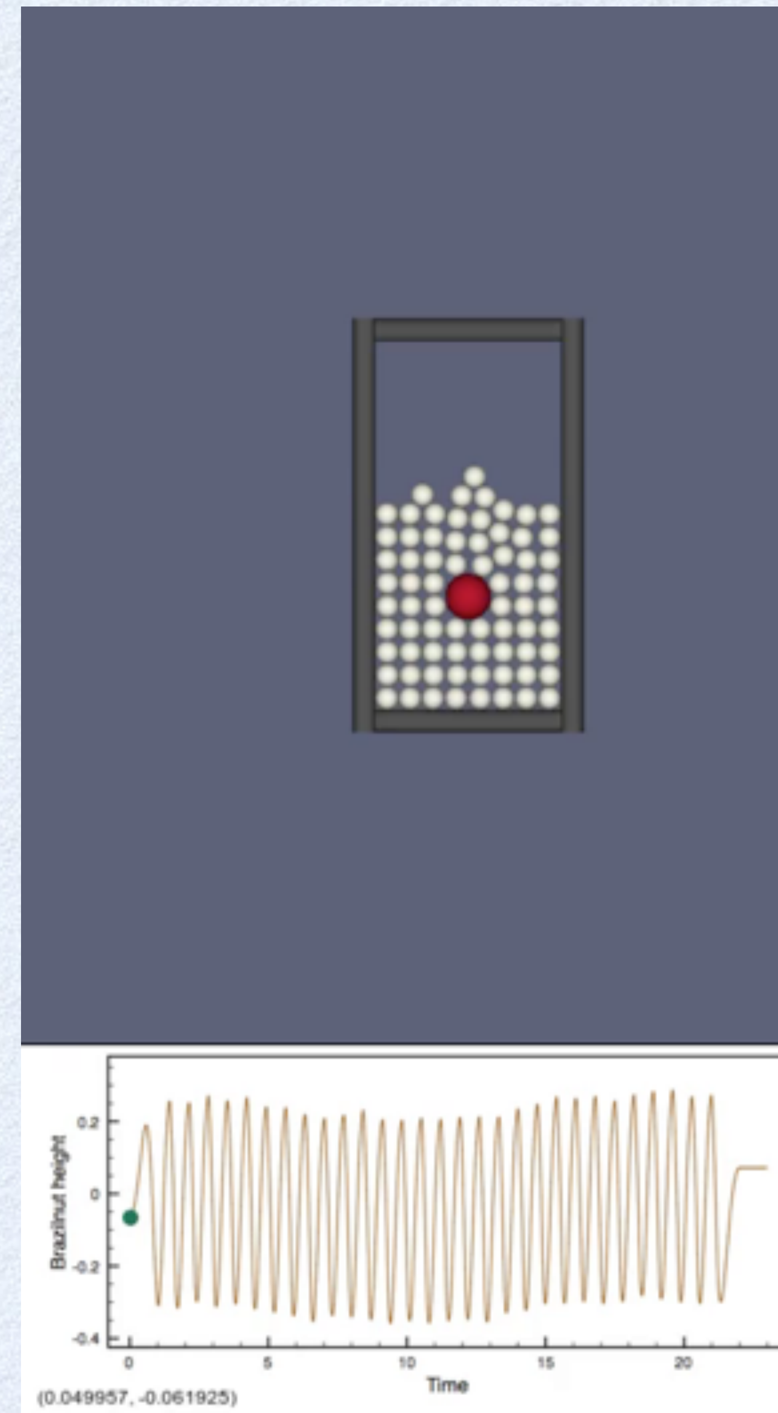
Simulations by CSE-LAB

[1] Cundall, Strack, Geotechnique, 1979



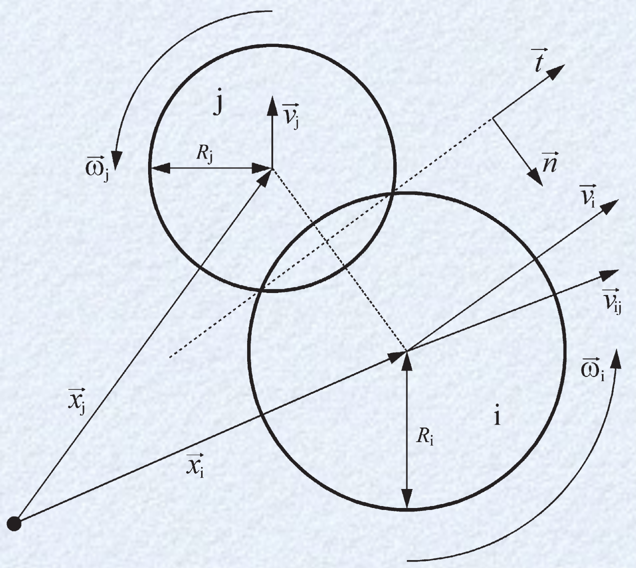


Fei Fang Chung et al. , Granular Material, 2009



Accelerating DEM

Catering for Many Particles : Evaluate the force-displacement interactions on the GPU, distribute the work on multiple nodes!



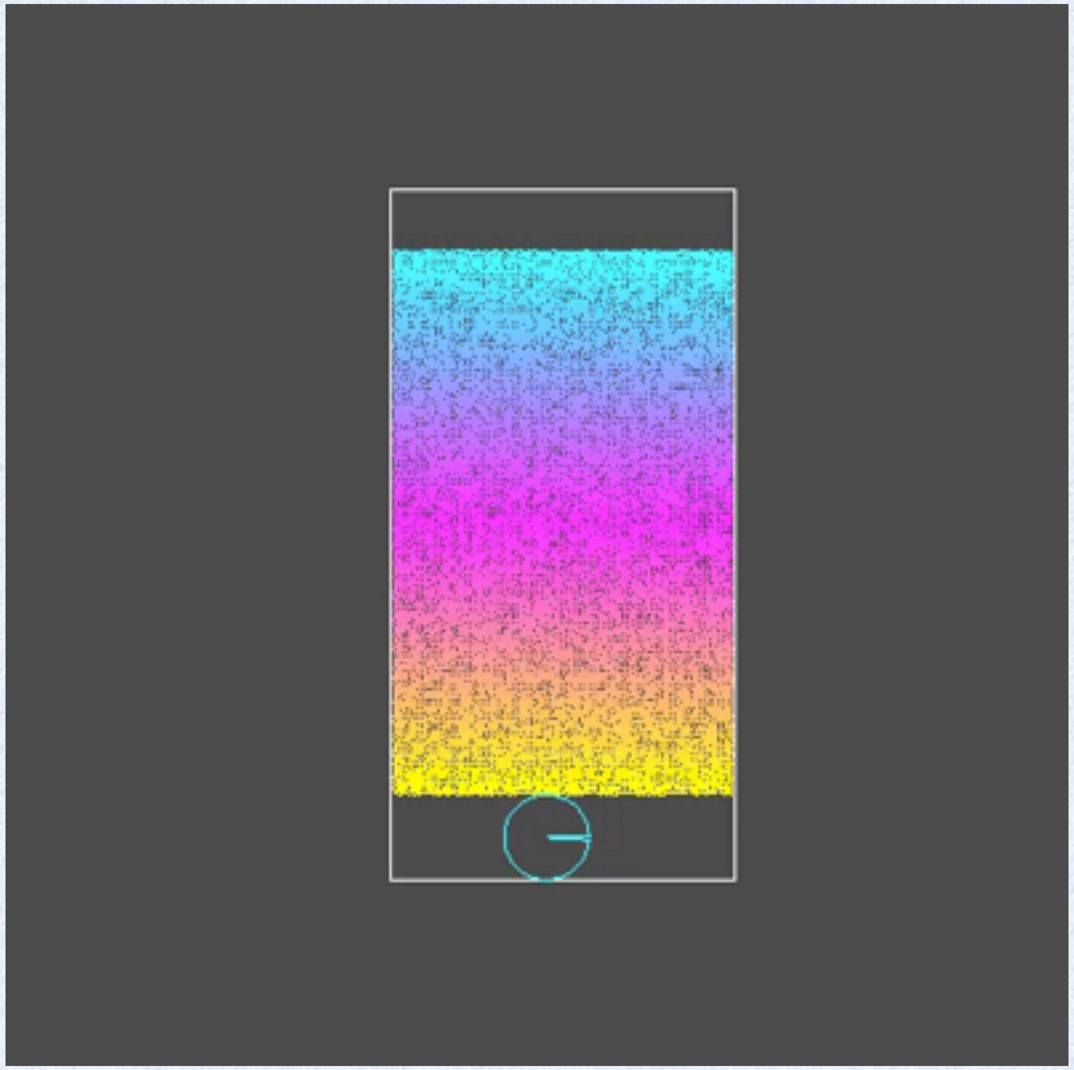
$$\mathbf{F}^n = -k^n \mathbf{y} - \gamma^n \frac{d\mathbf{y}}{dt} |\mathbf{y}|^{\Theta},$$

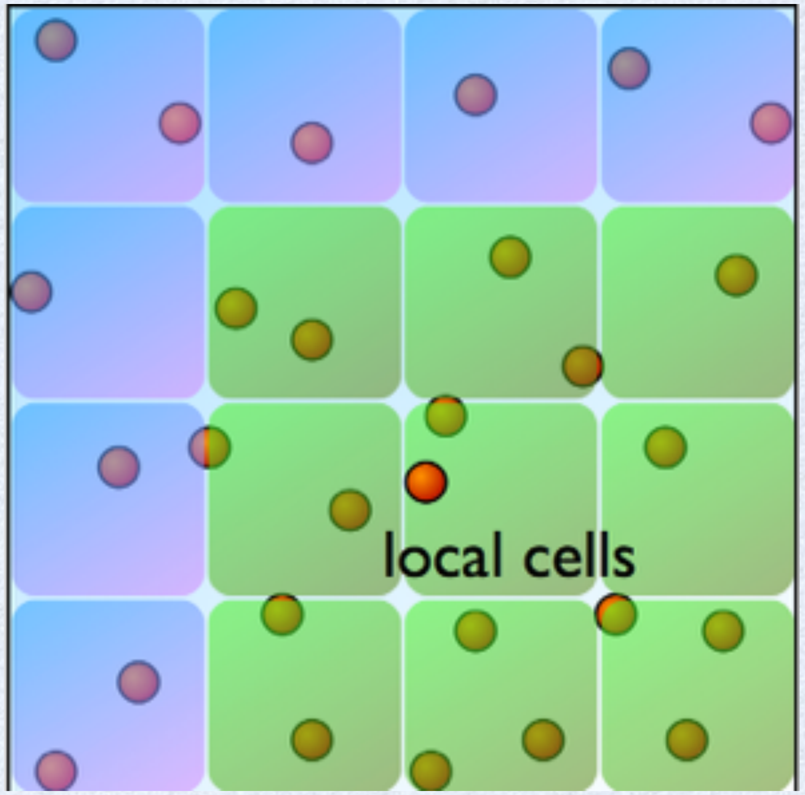
$$\mathbf{F}^t = \min\left(\frac{2}{3} k^s \boldsymbol{\xi}^t, \mu \mathbf{F}^n\right)$$

$$\boldsymbol{\xi}^t = \int_{t_0}^{t} \boldsymbol{v}_{rel}^t(\tau)\, d\tau,$$

$$k^n = \frac{4}{3} E_{eff} \sqrt{R_{eff}\,|\mathbf{y}|},$$

$$k^s = 8 G_{eff} \sqrt{R_{eff}\,|\mathbf{y}|}$$



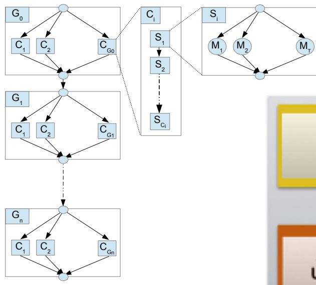


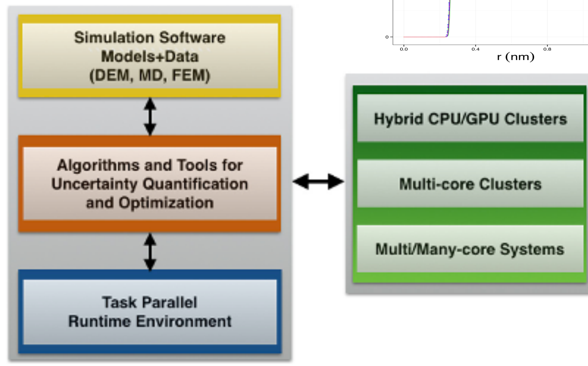
Take a look at the HPCSE I Project 1

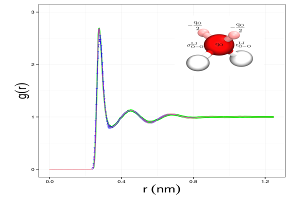
Uncertainty quantification

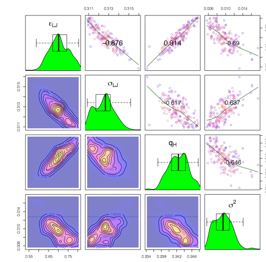
Diploma Thesis

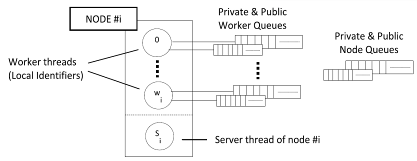
CHAIR OF COMPUTATIONAL SCIENCE

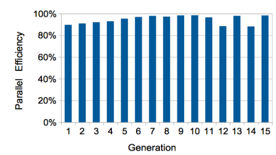


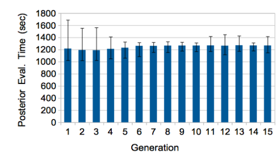












Parallel Uncertainty Quantification and Optimization Framework

Extension of the core layers of the Pi4U framework

Pi4U [1] is our in-house computational framework for large scale Bayesian uncertainty quantification (UQ) and stochastic optimization (SO) that can exploit massively parallel and hybrid (CPU/GPU) computing architectures.

The framework incorporates several state-of-the-art stochastic algorithms for the computation of the likelihood that are capable of sampling from complex, multimodal posterior distribution functions.

Built on top of the TORC task-parallel library, it offers straightforward extraction and exploitation of multilevel task-based parallelism in stochastic optimization and sampling algorithms.

Depending on his/her interests and background, the student can focus on:

(a) the development and study of algorithms for UQ and SO
(b) the extension and optimization of the framework on parallel architectures.

The evaluation can be performed using a wide range of scientific applications developed in our lab, without excluding applications proposed by the students.

This project is suitable for both Master and Bachelor level.

[1] www.cse-lab.ethz.ch/software/Pi4U

PREREQUISITES

Good Programming Skills (C/C++)
Desire to Learn and Improvise

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In the CSE Lab we combine computational methods, computer science tools and domain specific knowledge to solve scientific and Engineering Problems in areas such as Fluid Mechanics, Nanotechnology and Life Sciences. The core computational competences of our group are in particle methods and in stochastic optimization techniques.
Motivated by challenges in application fields, we focus on identifying the common elements among computational techniques and on formulating common methodological, algorithmic and software structures that facilitate their further development.