A Parallel Implicit Implementation of Smoothed Particle Hydrodynamics for Electrokinetic Applications

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Smoothed particle hydrodynamics (SPH)

Navier Stokes equations in Lagrangian form

$$\begin{cases} \dfrac{d\mathbf{u}}{dt} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{u}, \\ \nabla \cdot \mathbf{u} = 0, \\ \dfrac{d\mathbf{x}}{dt} = \mathbf{u}, \end{cases}$$

SPH Pros/Cons of Standard explicit SPH scheme

PROS: - no need to track boundaries
- amenable to parallelization
- good performance in high Reynold©number regimes

CONS: - accuracy (does not converge when increasing number of particles)
- performs poorly in low Reynold©number regimes
- particles need to be ªwellº distributed

In mesoscale applications, flows typically feature low Reynold©numbers

Standard explicit implementations would require tiny time steps, therefore we consider an **implicit** implementation.

Navier Stokes time discretization:

Implicit 2nd order incremental pressure correction

(improve performance for low Reynold©number flows)

Helmoltz system:
find velocity estimate

$$\begin{cases} \dfrac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = -\dfrac{1}{\rho}\nabla p^n + \dfrac{\nu}{2}\nabla^2\left(\mathbf{u}^* + \mathbf{u}^n\right) & x \in \Omega, \\ \mathbf{u}^* = 0 & x \in \partial\Omega, \end{cases}$$

Poisson system:
find pressure

$$\begin{cases} \dfrac{1}{\rho}\nabla^2 p^{n+1} = \dfrac{\nabla \cdot \mathbf{u}^*}{\Delta t} & x \in \Omega, \\ \partial_n p^{n+1} = 0 & x \in \partial\Omega. \end{cases}$$

Correct velocity
to make it
divergence free

$$\begin{cases} \dfrac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} = -\dfrac{1}{\rho}\nabla\left(p^{n+1} - p^n\right) & x \in \Omega, \\ \nabla \cdot \mathbf{u}^{n+1} = 0 & \\ \mathbf{u}^{n+1} \cdot \hat{n} = 0 & x \in \partial\Omega. \end{cases}$$

S. J. Cummins, M. Rudman, Journal of Computational Physics, 1999
S. M. Hosseini, J. J. Feng, 2011

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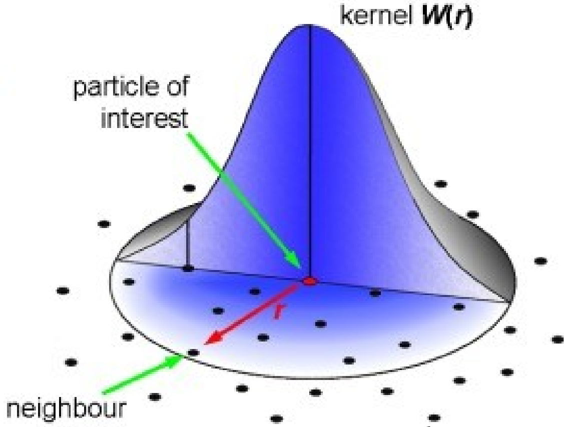
SPH discretization

Convolution with smooth kernel

$$\langle f \rangle(\mathbf{x}) = \int_{supp(W)} f(\mathbf{y}) W(\mathbf{x}-\mathbf{y}) d\mathbf{y}$$



www.nuigalway.ie

Compute derivatives differentiating the kernel

$$\langle \nabla f \rangle(\mathbf{x}) = \int_{supp(W)} f(\mathbf{y}) \nabla_{\mathbf{x}} W(\mathbf{x}-\mathbf{y}) d\mathbf{y}$$

Approximate integral as sum over particles

$$\widetilde{\nabla f}(\mathbf{x}_i) = \sum_{j \in supp(W)} f(\mathbf{x}_j) \nabla_{\mathbf{x}_i} W(\mathbf{x}_i - \mathbf{x}_j) V_j$$

volume fraction

Derive approximations for gradient operator and Lapalacian operator

$$\nabla_0 f_i = \sum_{j \in supp(W)} (f_j - f_i) \nabla_{\mathbf{x}_i} W_{ij} V_j \qquad \nabla_0^2 f_i = 2 \sum_{j \in supp(W)} \frac{f_i - f_j}{|\mathbf{r}_{ij}|} \mathbf{e}_{ij} \cdot \nabla_{\mathbf{x}_i} W_{ij} V_j$$

Zeroth order approximation

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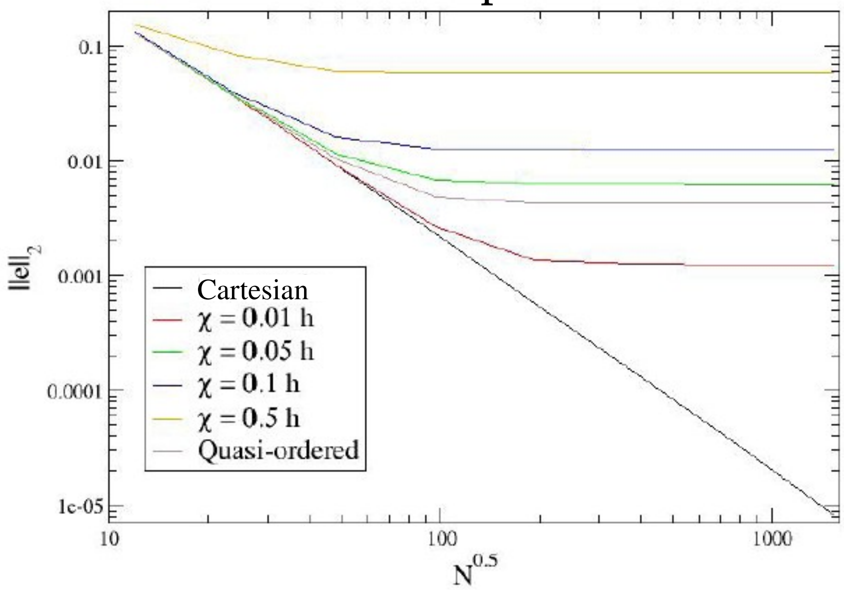
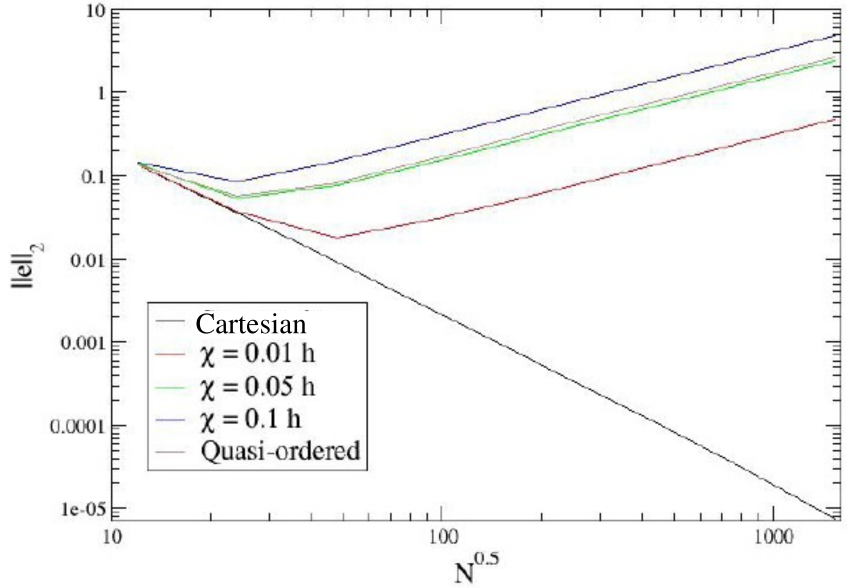
Zeroth order operators (in)accuracy

L2 error, for gradient and Laplacian operators applied on the function $u(x,y) = \sin(x)\sin(y)$, on different particles distributions (Cartesian, perturbed Cartesian, quasi-ordered).

Gradient operator



Lapalcian operator



χ : amount of uniformly distributed noise
h proportional $\sqrt{N}$ and to the kernel support radius

Convergence tests: N. Trask

Higher order SPH discretization

"standard" zeroth-order SPH discretization

$$\nabla_0 f_i = \sum_{j \in supp(W)} (f_j - f_i) \nabla_{\mathbf{x}_i} W_{ij} V_j$$

$$\nabla_0^2 f_i = 2 \sum_{j \in supp(W)} \frac{f_i - f_j}{|\mathbf{r}_{ij}|} \mathbf{e}_{ij} \cdot \nabla_{\mathbf{x}_i} W_{ij} V_j$$

"Corrected" first-order SPH discretization

$$\nabla_1 f_i = \sum_{j \in supp(W)} (f_j - f_i)\, \mathbf{G}_i \nabla_{\mathbf{x}_i} W_{ij} V_j$$

$$\nabla_1^2 f_i = 2 \sum_{j \in supp(W)} \left(\mathbf{L}_i : \mathbf{e}_{ij} \otimes \nabla_{\mathbf{x}_i} W_{ij}\right) \left(\frac{f_i - f_j}{|\mathbf{r}_{ij}|} - \mathbf{e}_{ij} \cdot \nabla_1 f_i\right) V_j$$

Correction tensors
(computed locally)

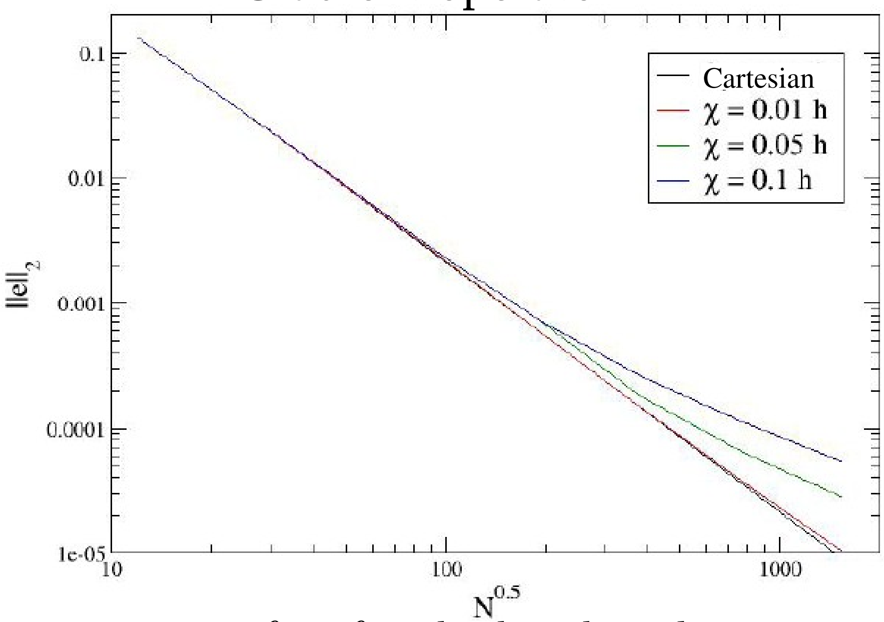
- "Almost" 2nd order accuracy
- Allows for fewer neighbors ➡ performance and scalability improvement

G. Oger et al, Journal of Computational Physics, 2007
R. Fatehi and M. T. Manzari, Computer and Mathematics with Application, 2011

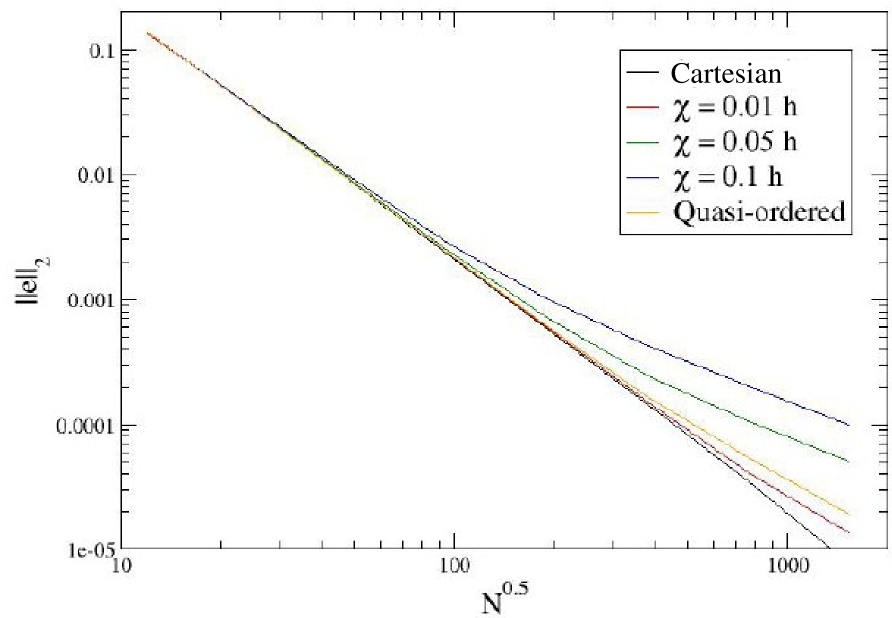
First-order operators accuracy

L2 error, for gradient and Laplacian operators applied on the function $u(x, y) = \sin(x)\sin(y)$ on different particles distributions (Cartesian, perturbed Cartesian, quasi-ordered).

Gradient operator



Lapalcian operator



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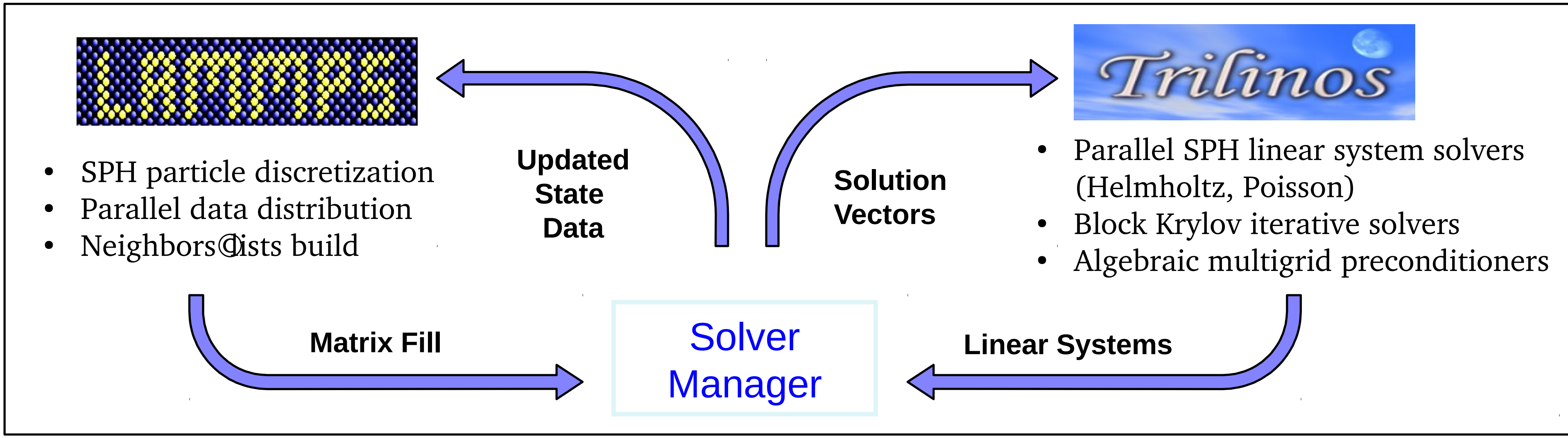
Convergence tests: N. Trask

SPH implementation



Fuse LAMMPS and Trilinos for massively parallel 3D SPH computational framework

Let each code handle what it was designed to do well

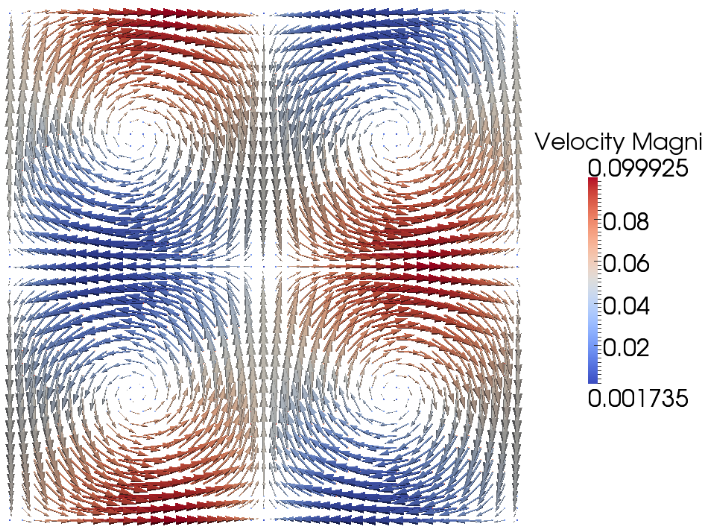
- LAMMPS handles particle data, parallel data distribution, neighboring
- Trilinos handles distributed memory linear/nonlinear solvers, preconditioners, etc.

N. Trask et al, CMAME, submitted, 2014

Scalability results for 3D Taylor-Green Vortex

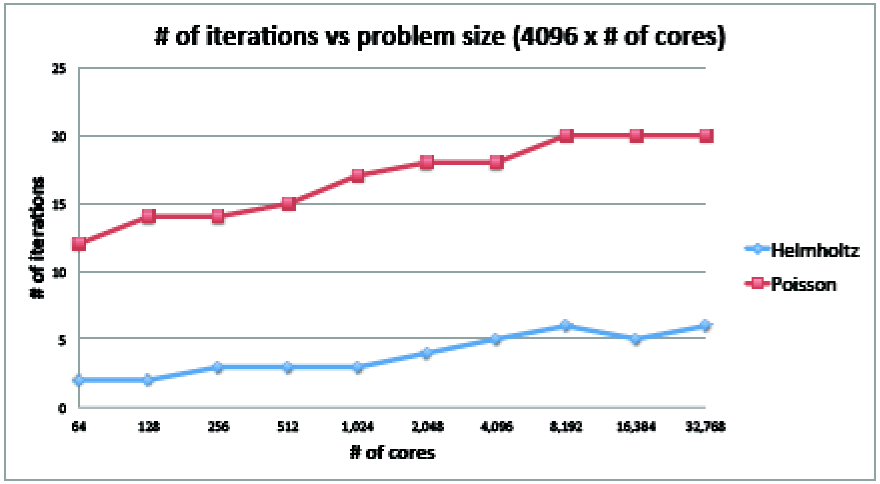
Synthetic problem
manufactured solution:

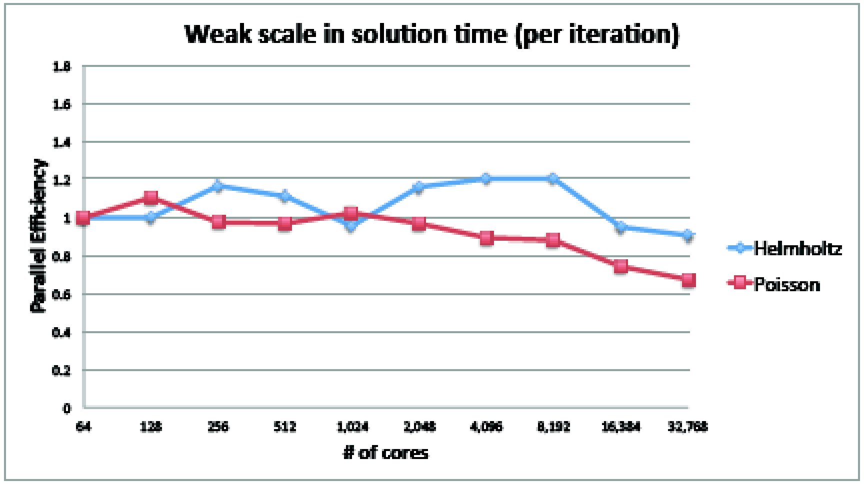
$$u_x = U_0 e^{-2\nu\pi^2 t}\sin(\pi x)\cos(\pi y)$$
$$u_y = -U_0 e^{-2\nu\pi^2 t}\cos(\pi x)\sin(\pi y)$$
$$p = \frac{U_0^2}{4} e^{-4\nu\pi^2 t}(\cos(2\pi x) + \cos(2\pi y) + 2)$$



t = 0.000

Scalability results using up to 134 millions particles and 32K cores





To our knowledge, the largest implicit SPH simulation ever

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Verification with Finite Volume for BCC lattice

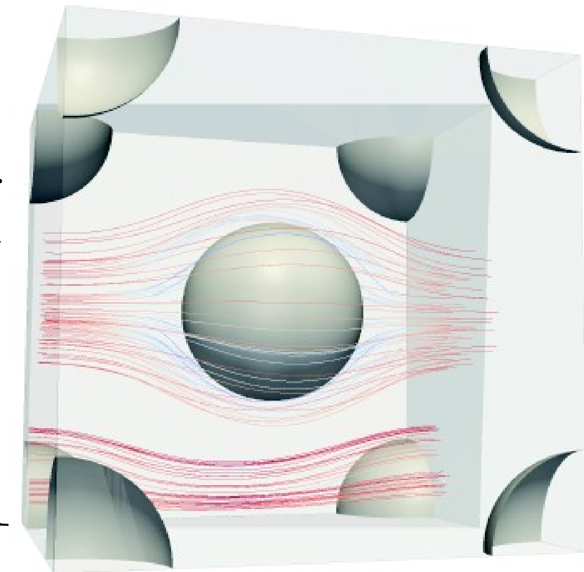
Problem details:

No slip boundary conditions:
Morris/Holmes Dirichlet boundary conditions to provide $^{a}2^{nd^{o}}$ accuracy

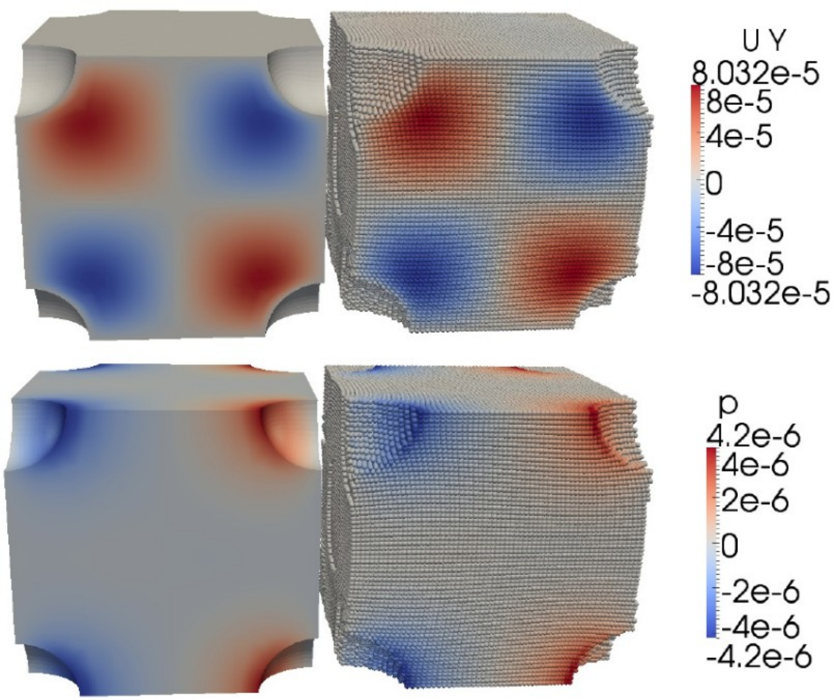
OK for complex geometries
(no need to have analytic representation of boundaries)

Streamlines colored with magnitude of velocity

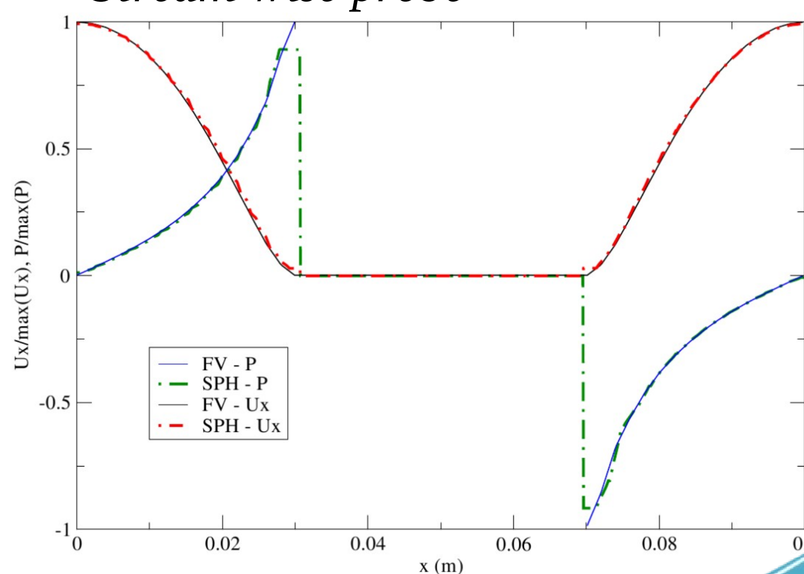
$$Re \simeq 0.1$$



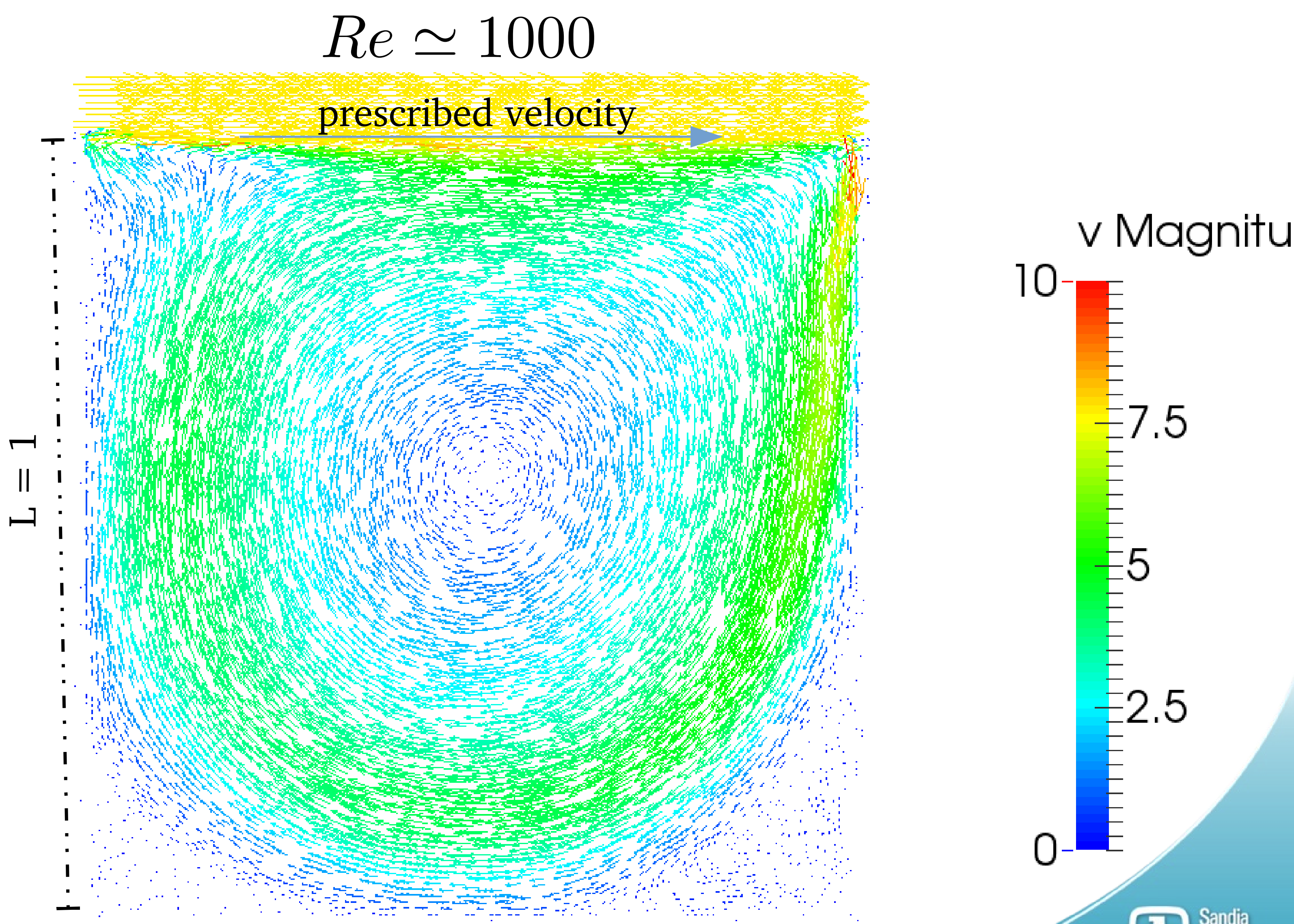
Comparison with finite volumes



Stream-wise probe

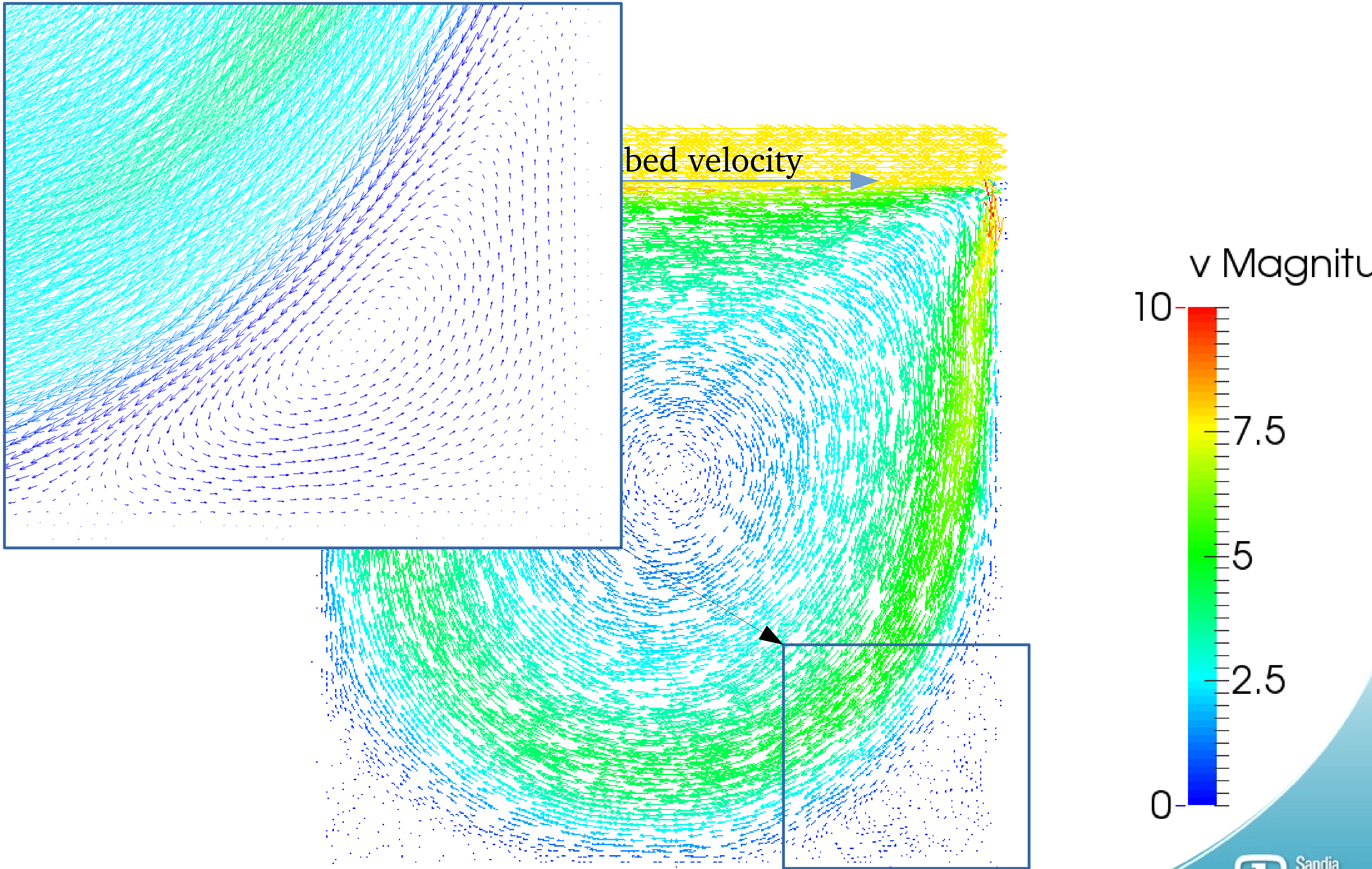


Navier Stokes numerical benchmarks
lid driven cavity



simulation: K. Kim

Navier Stokes numerical benchmarks
lid driven cavity



simulation: K. Kim

Towards electrokinetic problems: Poisson Boltzmann equation

Boltzmann charge distribution for a **two-ion monovalent** system: $\boxed{c^{\pm} = \pm c_b \exp(\mp\tilde{\psi})}$

Nonlinear Poisson-Boltzmann equation:

$$\boxed{-\nabla^2\tilde{\psi} = -\kappa^2 \sinh\tilde{\psi}, \qquad \text{with } \kappa^2 := 2\frac{c_b e^2}{\epsilon K_B T}}$$

Elctrokinetic ***forcing term*** appearing in the Navier Stokes equation

$$\boxed{\rho\,\mathbf{f} = 2\,e\,c_b\,\psi_{th}\,\sinh(\tilde{\psi})\,\nabla\tilde{\psi}}$$

Polarized fluid is driven by electric potential

Implementation uses SPH Laplacian operator introduced before
Nonlinearity solved with Newton method (NOX package in Trilinos)

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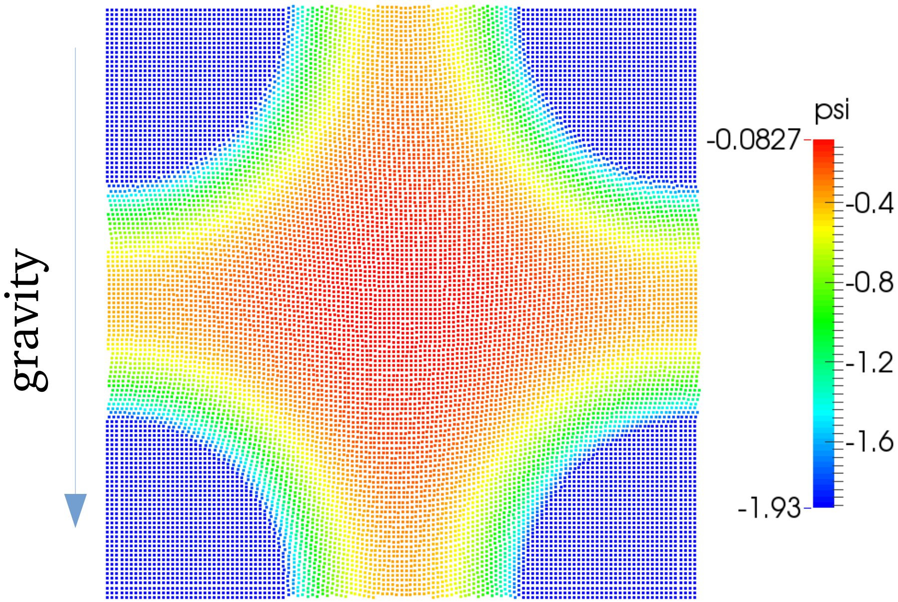
Benchmarks on electrokinetic effect

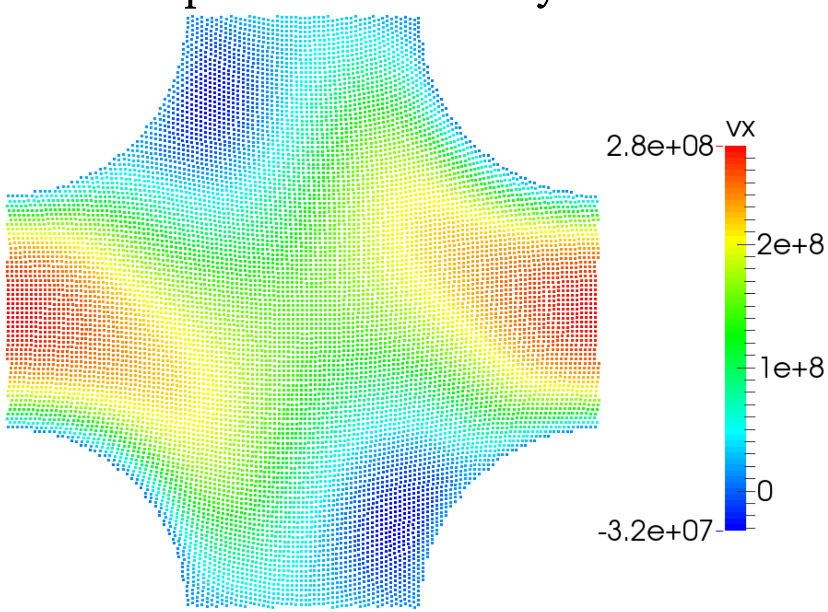
potential field



Four corners has fixed negative potential
Gravity field is prescribed

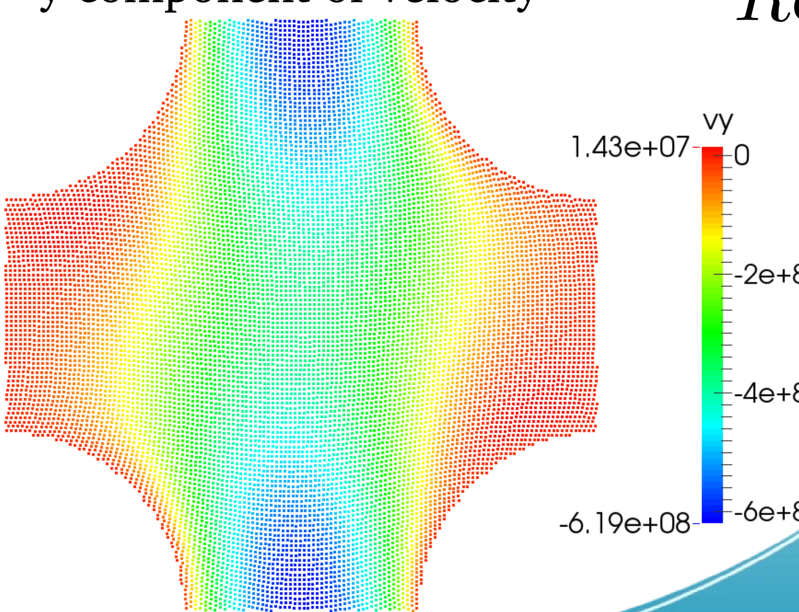
The electric potential clearly perturb the gravity driven flow

x component of velocity



y component of velocity

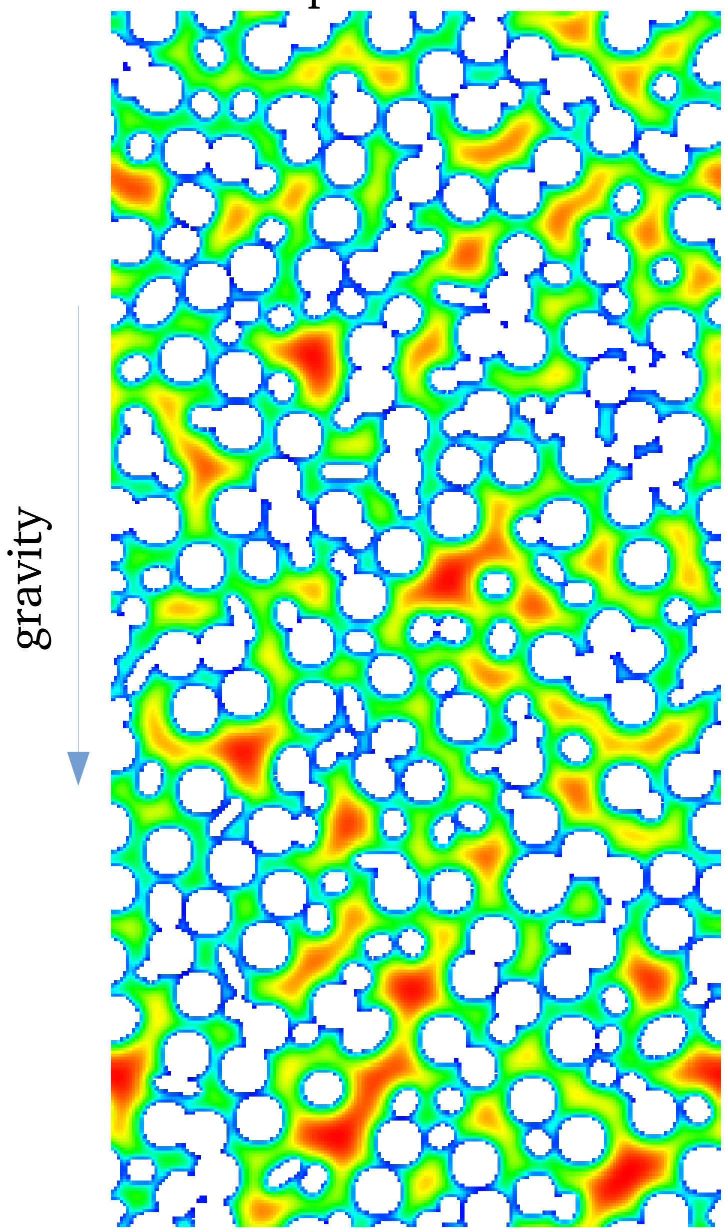
$$Re \simeq 0.02$$



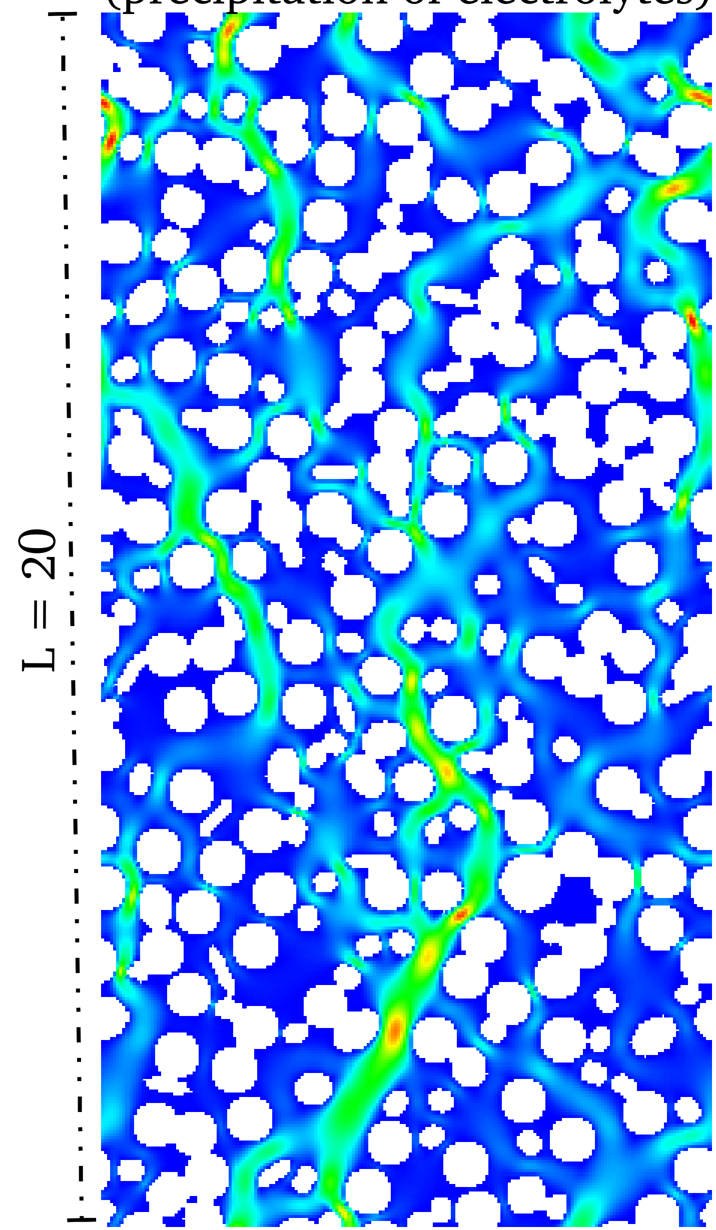
Problem setting: W. Pan, simulation: K. Kim

Li-air batteries application

potential



velocity magnitude
(precipitation of electrolytes)



Used first order time scheme to prevent oscillations

$$Re \simeq 10^{-7}$$

Problem setting: W. Pan, simulations: K. Kim

On-going / future developments

- Improve scheme stability for very low Reynolds numbers
- Use high-order mesh-free schemes (e.g. MLS)
- Design high order conservative schemes
- Improve model fidelity using Poisson-Nerst-Planck equations and/or use DFT (density functional theory)
- Solve new problems, e.g. microfluidic mixing

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