# CASL: Computational Applied Science Laboratory

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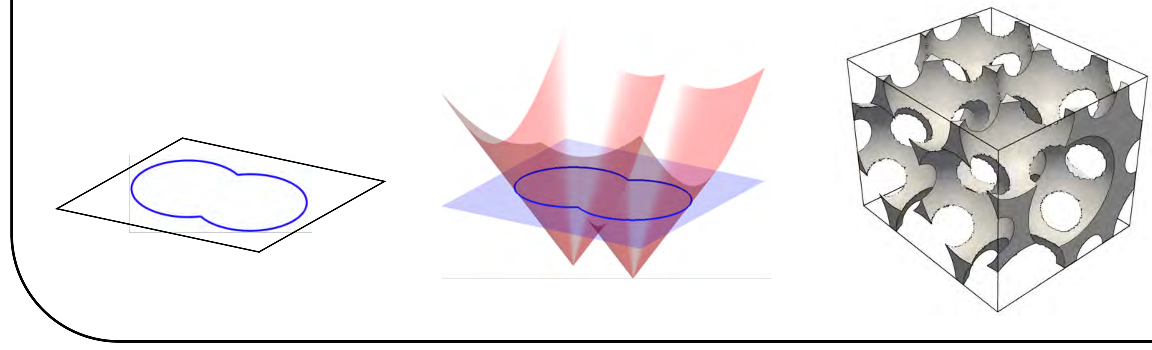
## Abstract

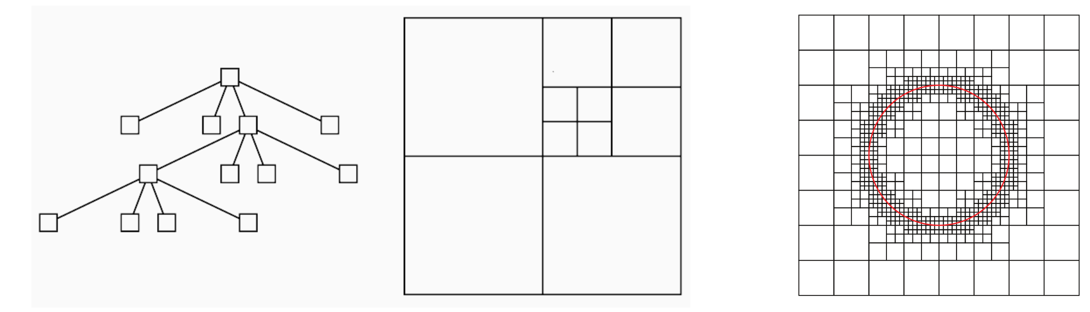
- Accurate simulations and predition of complex physical phenomena can lead to leap-frog technology in science and engineering.
- We develop and apply robust, versatile numerical algorithms that enable the solution of scientific problems that are otherwise intractable.
- Our computational methods address the following challenges:
  - Irregular geometries and free boundary problems
  - Spatially multiscale and multiphysics problem
  - Development and implementation of parallel algorithms

## Computational Framework

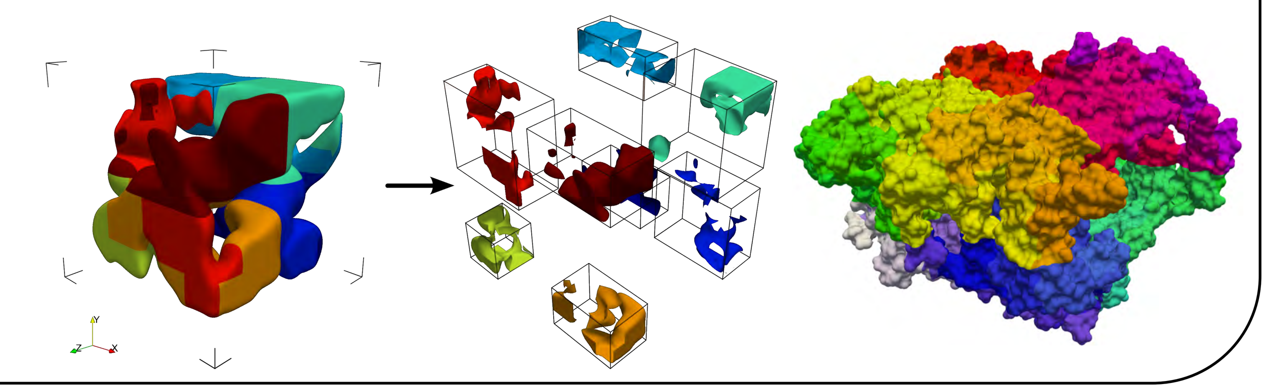
- Novel finite difference and finite volume algorithms based on adaptive Cartesian grids.
- Complex boundaries are represented implicitly which enables:
  - Automatic and efficient grid generation.
  - Robust handling of moving interfaces.
  - Easy implementation of boundary conditions



- Octree (3D) and quadtree (2D) data-structures are used to efficiently store adaptive grids.
- Grid refinement/coarsening is performed automatically be defining a refinement criteria (e.g. distance from the boundary)



- Both shared (OpenMP) and distributed (MPI) memory as well as GPGPU (CUDA) techniques are utilized to enable fast and efficient solution to very large scientific problems.



## Incompressible Fluid Dynamics

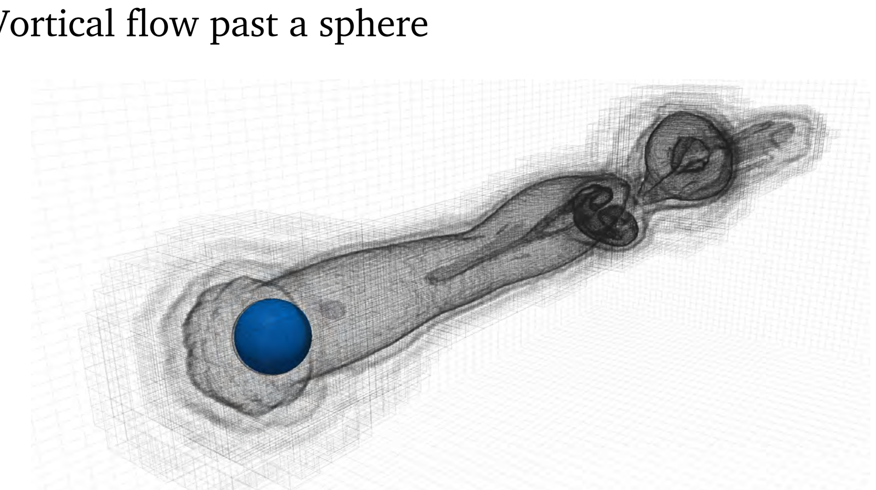
- Complex vortical flows
- Thin boundary layers
- The physics are described by the viscous, incompressible Navier-Stokes equations:

$$\rho(\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u}) = -\nabla p + \mu\Delta\mathbf{u} + \mathbf{f}$$

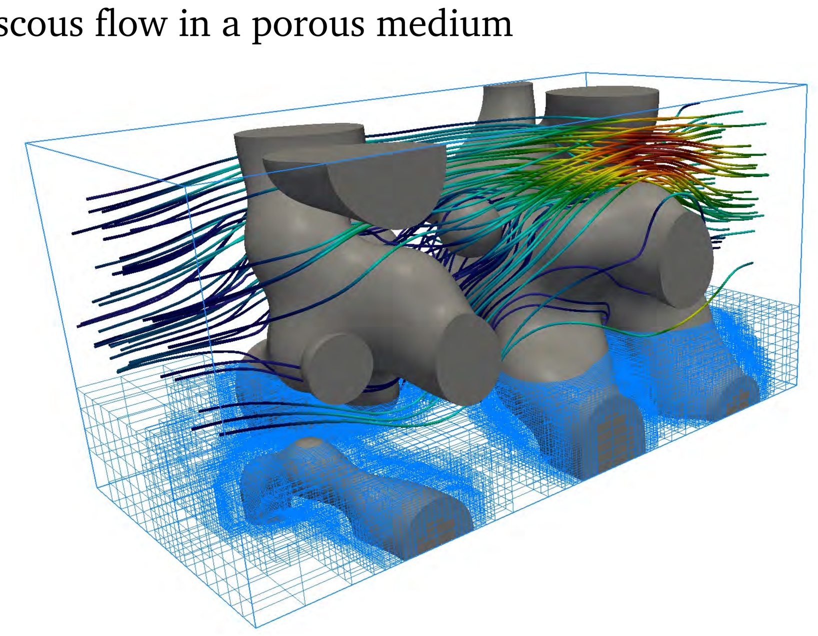
$$\nabla\cdot\mathbf{u} = 0$$

| | |
|---|---|
| $\mathbf{u}$ | Velocity vector |
| $p$ | Pressure |
| $\rho$ | Density |
| $\mu$ | Viscosity |
| $\mathbf{f}$ | External forces |

- Example of complex three dimensional applications
  - Vortical flow past a sphere

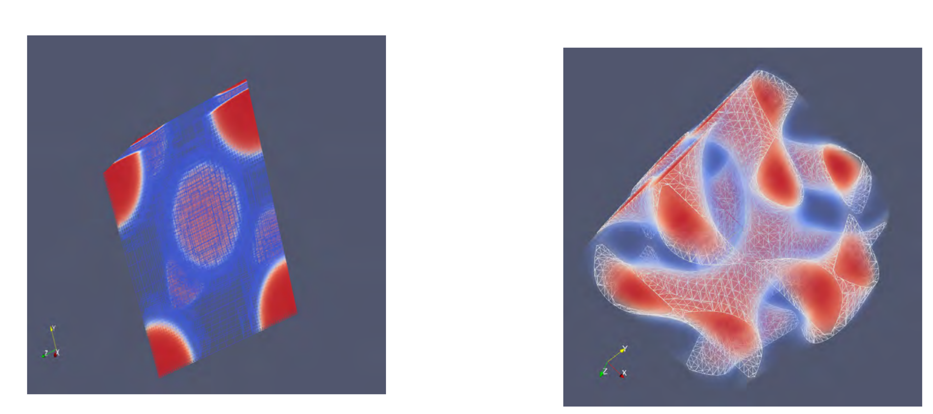


  - Viscous flow in a porous medium

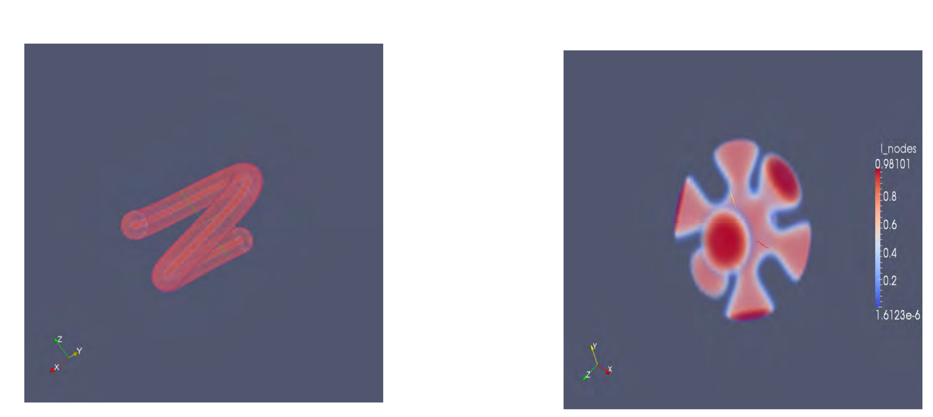


## Polymer Statistical Physics

- Global Optimization to find the polymer structure at equilibrium.
- The optimization is an iterative solver on a highly non-linear functional. At each optimization iteration diffusion equation describing the polymer probability has to be solved.
- Seed a field $\omega$
  while $(||\delta H/\delta\omega||_2 < \epsilon)$
  - solve a diffusion equation: $\frac{\partial q}{\partial t} = \frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2} + \frac{\partial^2 q}{\partial z^2} - (q \times w)$ from t=0 to t=1 with T=1/dt diffusion iterations.
  - compute the densities $\rho_a, \rho_b$
  - compute the forces
  - advance the potential $\omega$ up to the functional optimization algo
  - compute energy and check convergence criterions
- Bcc and Gyroid in the bulk



- Confined Domains



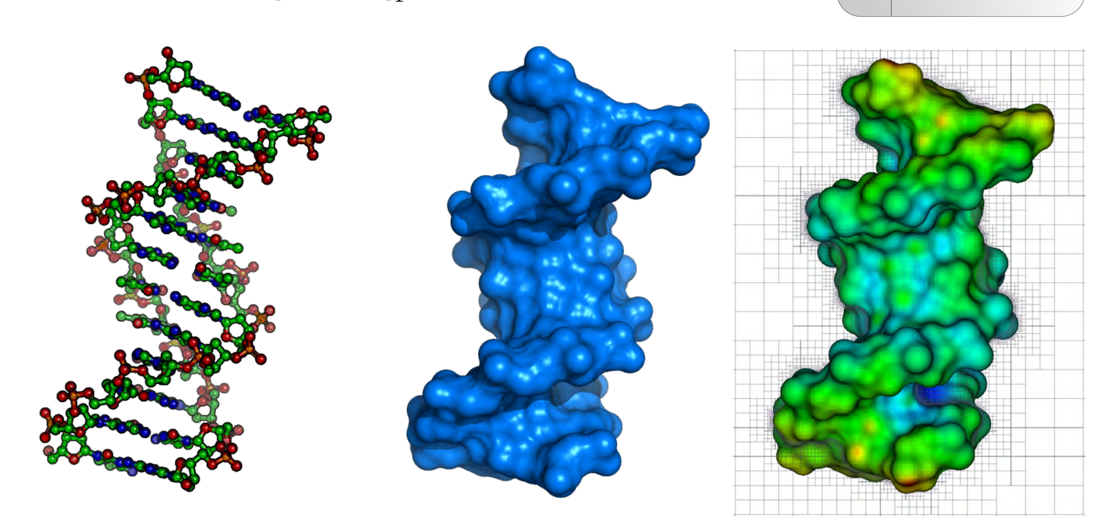
## Nano-scale Electrochemistry

- Electrostatic calculations is at the heart of many electrochemical problems at the nano-scale.
- Electrostatic distribution around charged molecules is described via the nonlinear Poisson-Boltzmann equation.

$$-\nabla\cdot(\epsilon\nabla\psi) + \kappa^2(\mathbf{x})\sinh(\psi) = \sum_{i=1}^{N_m} z_i\delta(\mathbf{x}-\mathbf{x}_i)$$

$$[\psi]_\Gamma = 0, \qquad [\epsilon\nabla\psi\cdot\mathbf{n}]_\Gamma = 0.$$

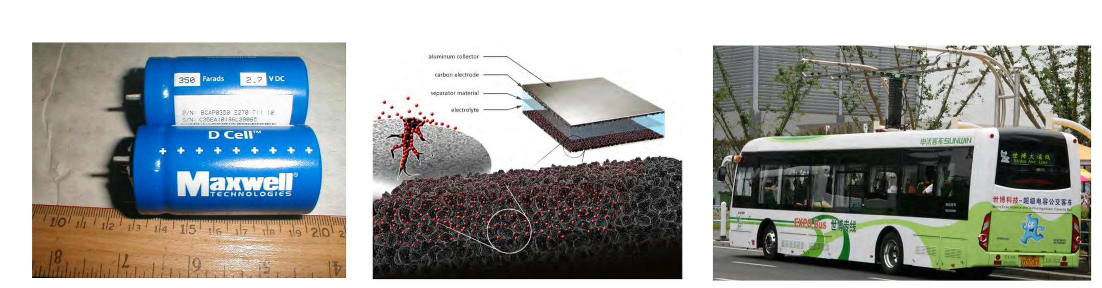
| | |
|---|---|
| $\psi$ | Electrostatic Potential |
| $\epsilon$ | Dielectric constant |
| $\kappa$ | Inverse Debye Length |
| $z_i$ | Ion valence |

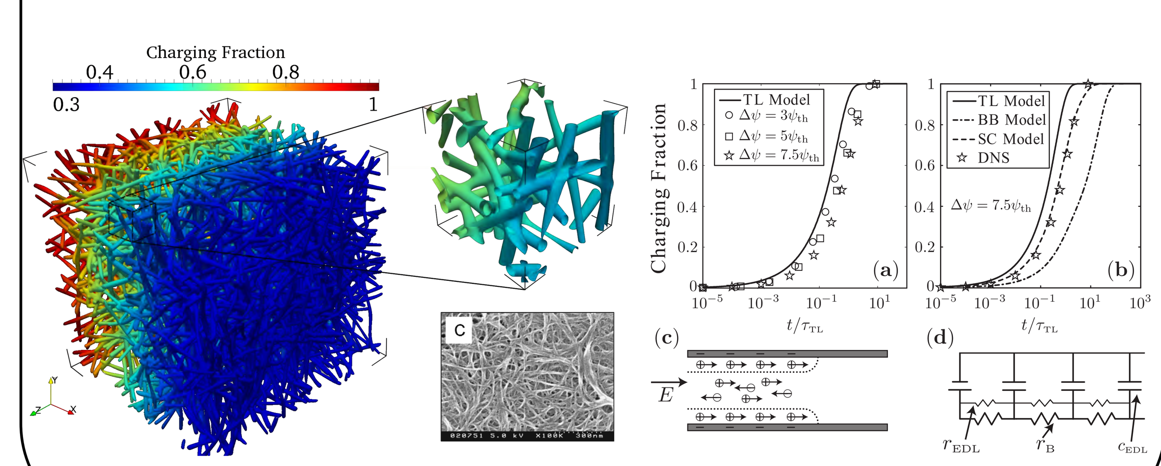


- Supercapacitors may be studied by solving the Poisson-Nernst-Planck equations:

$$\begin{aligned}\partial_t c_+ &= \nabla^2 c_+ + \nabla\cdot(c_+\nabla\psi)\\ \partial_t c_- &= \nabla^2 c_- - \nabla\cdot(c_-\nabla\psi)\\ \nabla^2\psi &= -\kappa^2(c_+ - c_-)\end{aligned}$$

| | |
|---|---|
| $c_+$ | Cation Concentration |
| $c_-$ | Anion Concentration |
| $\psi$ | Electric potential |
| $\kappa$ | Ratio of bulk length scale to Debye layer thickness |

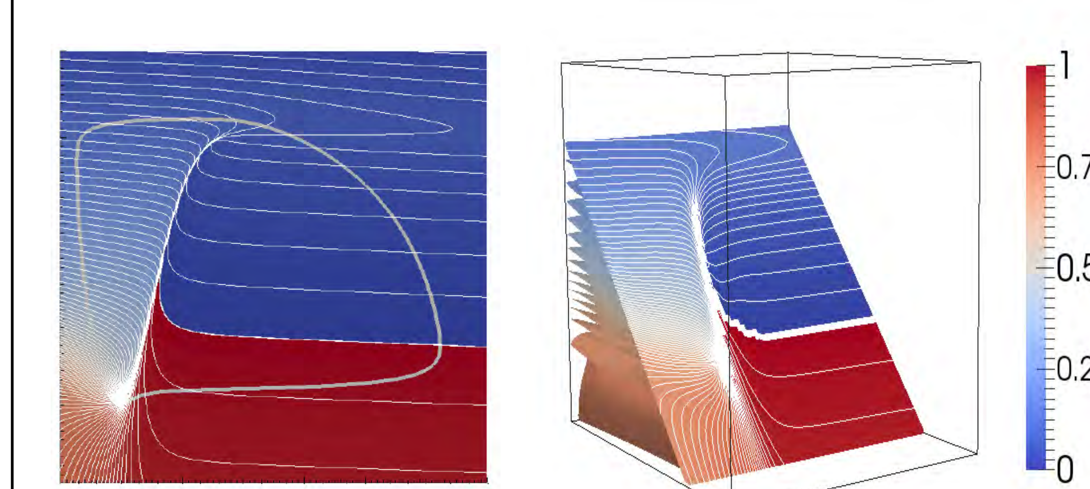


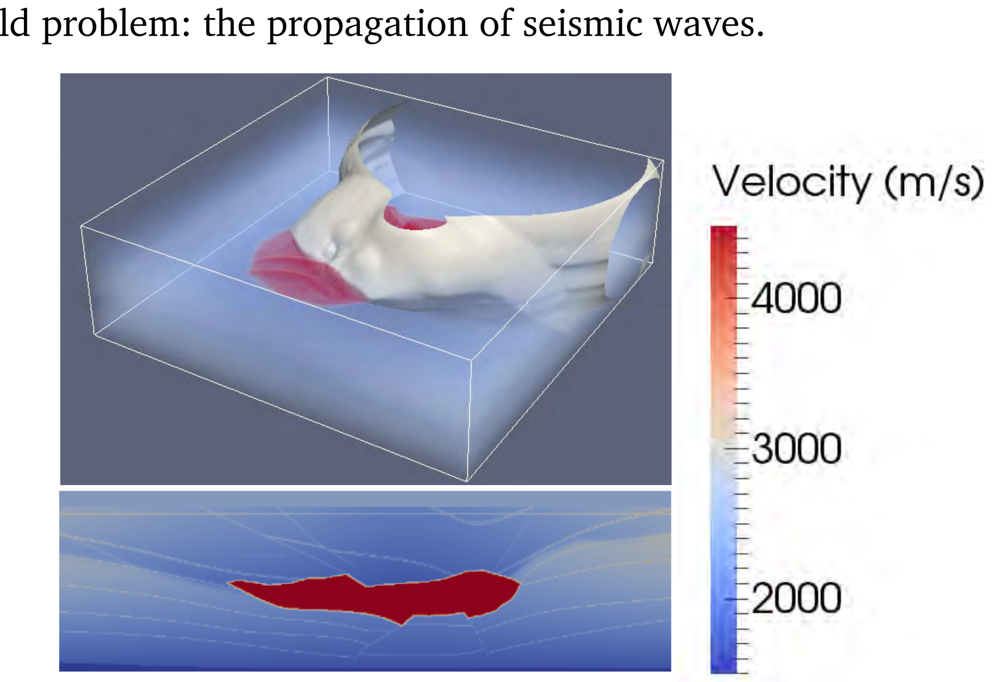

## Parallel Fast Sweeping

- The fast sweeping method (FSM) can be used to solve many Hamilton-Jacobi problems.
- Our novel parallel algorithms coupled with hybrid parallel computing clusters allow us to study new problems and existing problems in much finer detail than before.
- New problem: computing "isochrons" of a dynamical system.

$$\begin{aligned}\nabla\theta\cdot\mathbf{F}(\mathbf{x}) &= \frac{2\pi}{T_\Gamma} \quad \forall\,\mathbf{x}\in\mathcal{B},\\ \theta(\gamma) &= f(\gamma) \quad \forall\,\gamma\in\Gamma^+,\end{aligned}$$




- We study the phase dynamics of a human neuron.
  - This can help to develop desynchronizing controls, a possible treatment for Parkinson's disease.
- Old problem: the propagation of seismic waves.




- Elastic wave traversing a natural salt dome formation. Can solve this problem on huge grids (billions of cells).