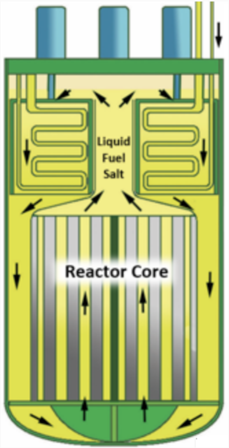
Spectral Element Methods for Coupled PNP-NS equations

Yimin Lin, Paul Fischer, Haomin Yuan, Misun Min

Department of Computational and Applied Mathematics, Rice University
Mathematics and Computer Science Division, Argonne National Laboratory
Department of Computer Science, University of Illinois at Urbana-Champaign
Nuclear Science and Engineering Division, Argonne National Laboratory

Motivation: Molten Salt Reactors

- Numerical simulations of molten salt reactor



Molten salt reactor

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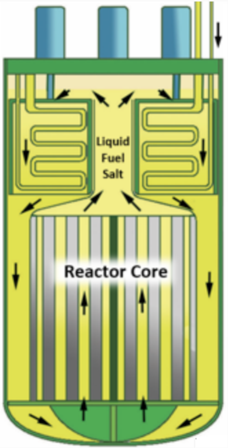
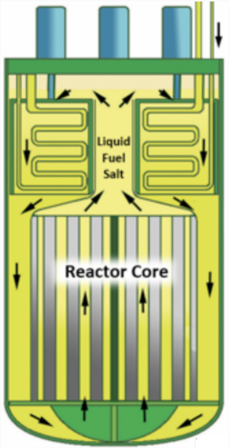
- Numerical simulations of molten salt reactor
- Charge neutrality leads to a different mass transfer mechanism



Molten salt reactor

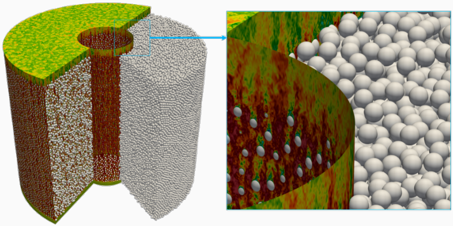
Motivation: Molten Salt Reactors

- Numerical simulations of molten salt reactor
- Charge neutrality leads to a different mass transfer mechanism
- Corrosion by electrochemical reactions on surfaces



Molten salt reactor

- Physical phenomena governed by PDE: nuclear reactors

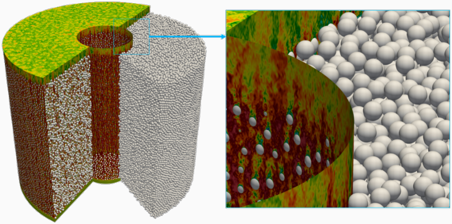


NekRS run on 27648 GPUs on Summit for a full-core pebble-bed reactor with 352625 pebbles [1]

[1] Lan et al., "All-Hex Meshing Strategies For Densely Packed Spheres", 2021

High Order Spectral Element Methods for PDEs

- Physical phenomena governed by PDE: nuclear reactors
- More accurate per degrees of freedom than low order methods (for smooth solutions), low dispersion error



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High Order Spectral Element Methods for PDEs

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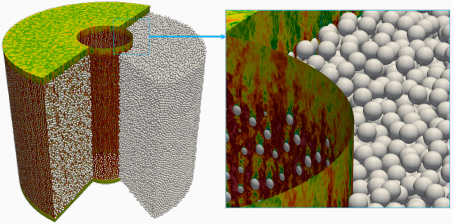
- More accurate per degrees of freedom than low order methods (for smooth solutions), low dispersion error
- Nek5000/NekCEM/NekRS: scalable spectral element solver on CPU and GPGPU



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Governing Equation

- Coupled system of incompressible Navier-Stokes and PNP (Poisson-Nernst-Planck) equations

$$
Fluid \begin{cases}
\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p - \frac{1}{Re} \nabla^2 \boldsymbol{u} & = g\left(T, c\right) \\
\nabla \cdot \boldsymbol{u} & = 0 \\
\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \nabla T & = \nabla \cdot \left(\frac{1}{Re \cdot Pr} \nabla T + \sum \frac{Q_i}{Re \cdot Sc_i} \nabla c_i \right)
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$$
\textit{Ion} \quad \begin{cases} \frac{\partial c_i}{\partial t} + \nabla \cdot \left(\boldsymbol{N}_i + c_i \boldsymbol{u} \right) &= 0 \\ \sum_i z_i c_i &= 0 \end{cases}
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Electroneutrality condition

- Finite element discretization, fully implicit nonlinear solve [2]

$$\mathcal{R}^{n+1}\left(\begin{bmatrix} c_1^{n+1} \\ \vdots \\ c_{N_c}^{n+1} \\ \phi^{n+1} \end{bmatrix}\right) = \begin{bmatrix} \mathcal{R}_1^{n+1}\left(c_1^{n+1}, \phi^{n+1}\right) \\ \vdots \\ \mathcal{R}_{N_c}^{n+1}\left(c_{N_c}^{n+1}, \phi^{n+1}\right) \\ \sum z_i c_i^{n+1} \end{bmatrix} = \mathbf{0}$$

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- Decouples through Poisson solve

$$\sum z_i c_i = 0 \qquad \Longrightarrow \qquad \nabla \cdot \left(\sum z_i^2 c_i \nabla \phi\right) = \nabla \cdot \left(\sum \frac{z_i}{Re \cdot Sc_i} \nabla c_i\right)$$

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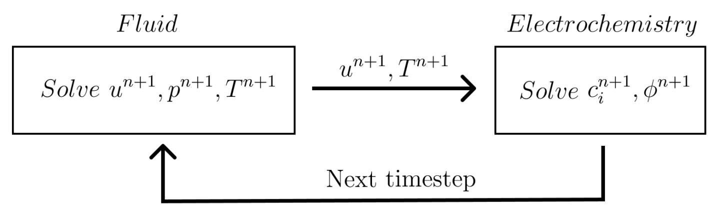
Numerical Discretization

- Decouple complex physics through semi-implicit timestepping



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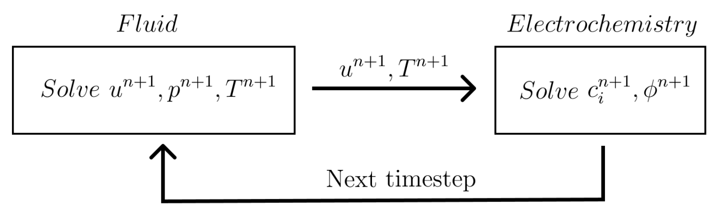

- Weak form of PNP equations, for all $v, w \in X_0^N$

$$\frac{d}{dt}(v, c_i) - (\nabla v, \frac{1}{Re \cdot Sc_i}\nabla c_i) = (\nabla v, \frac{1}{Re \cdot Sc_i} z_i c_i \nabla \phi + \frac{1}{Re \cdot Pr} Q_i c_i \nabla T),$$

$$-(\nabla w, z_i^2 c_i \nabla \phi) = (\nabla w, \sum \frac{z_i}{Re \cdot Sc_i} \nabla c_i)$$

Temporal Discretization

- Temporal Discretization: semi-implicit BDF-k/EXT-k

$$\frac{d}{dt}(v, c_i) - (v, \nabla \cdot (\frac{1}{Re \cdot Sc_i} \nabla c_i)) = (\nabla v, \frac{1}{Re \cdot Sc_i} z_i c_i \nabla \phi + \frac{1}{Re \cdot Pr} Q_i c_i \nabla T),$$

$$-(w, \nabla \cdot (z_i^2 c_i \nabla \phi)) = (\nabla w, \sum \frac{z_i}{Re \cdot Sc_i} \nabla c_i)$$

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$$
\begin{aligned}
\sum_{j=0}^{k} \frac{\beta_j}{\Delta t}(v, c_i^{n-j}) - (\nabla v, \frac{1}{Re \cdot Sc_i} \nabla c_i^n) &= (\nabla v, r^n), \\
-(\nabla w, z_i^2 c_i^n \nabla \phi^n) &= (\nabla w, f^n),
\end{aligned}
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$$-(\nabla w, z_i^2 c_i^n \nabla \phi^n) = (\nabla w, f^n),$$

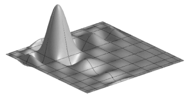
- k-th order extrapolation of nonlinear terms

$$r^n = \sum_{j=1}^{k} \alpha_j \left[\frac{1}{Re \cdot Sc_i} z_i c_i^{n-j} \nabla \phi^{n-j} + \frac{1}{Re \cdot Pr} Q_i c_i^{n-j} \nabla T^{n-j} \right],$$

$$f^n = \sum_i \sum_{j=1}^{k} \alpha_j \frac{z_i}{Re \cdot Sc_i} \nabla c_i^{n-j}$$

Spatial Discretization

- Spatial Discretization: Spectral element, Tensor products of high order Lagrange interpolation polynomial on LGL nodes.



2D basis function, N=10

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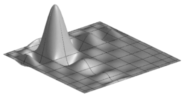

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$$D = I \otimes I \otimes \widehat{D}$$

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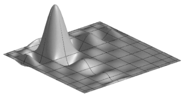

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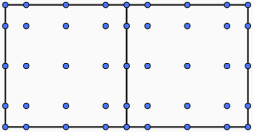
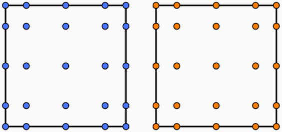
- Matrix assembly and continuity enforcement

$$\int_{\Omega} \frac{\partial u}{\partial t} = \int_{\Omega} \mathcal{L}(u), \mathsf{M}\frac{\partial \mathsf{u}}{\partial t} = \mathsf{L}\mathsf{u} \quad \Longrightarrow \quad \int_{\Omega^e} \frac{\partial u}{\partial t} = \int_{\Omega^e} \mathcal{L}(u), \mathsf{M}^e\frac{\partial \mathsf{u}}{\partial t} = \mathsf{L}^e\mathsf{u}$$



Global Representation



Local Representation

Electrokinetics boundary condition

- Butler-Volmer boundary condition

$$\boldsymbol{N}_i \cdot \boldsymbol{n} = \frac{i\left(c_i, \phi\right)}{z_i F}, \quad i\left(c_i, \phi\right) = i_0 c_i^{\gamma}\left[\exp\left(\epsilon\left(V - \phi\right)\right) - \exp\left(-\epsilon\left(V - \phi\right)\right)\right]$$

[3] Newman and Thomas-Alyea, *Electrochemical systems*.

[4] Doche, Bauer, and Tardu, “Direct Numerical Simulation of an electrolyte deposition under a turbulent flow–A first approach”, 2011

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- Current density doesn't change at thin diffusion layer at the electrode[3]

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- Current density doesn't change at thin diffusion layer at the electrode[3]

$$\frac{\partial \phi}{\partial n} = i(c_i, \phi)$$

- Given the equilibrium potential, reduce to a single Newton solve:

$$\phi = E^{eq}, \quad \int_{\partial \text{electrodes}} \boldsymbol{N}_i \cdot \boldsymbol{n} = 0$$

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- Linearization of Butler-Volmer reduces to the Robin boundary condition [4]

[3] Newman and Thomas-Alyea, *Electrochemical systems*.

[4] Doche, Bauer, and Tardu, "Direct Numerical Simulation of an electrolyte deposition under a turbulent flow–A first approach", 2011

Convergence Test

- Construct exact solution by introducing source terms

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \frac{1}{Re}\Delta \boldsymbol{u} + \sum_{i=1}^{2} \gamma_i c_i \boldsymbol{g} + \boldsymbol{f},$$

$$\nabla \cdot \boldsymbol{u} = 0,$$

$$\frac{\partial c_i}{\partial t} + \boldsymbol{u} \cdot \nabla c_i = \frac{1}{Pe} D_i \Delta c_i + \frac{1}{Pe} \nabla \cdot (z_i D_i c_i \nabla \phi) + h_i$$

$$-\nabla \cdot (\sum_{i=1}^{2} D_i c_i \nabla \phi) = \nabla \cdot \left(\sum_{i=1}^{2} z_i D_i \nabla c_i \right),$$

- Exact solution:

$$\boldsymbol{u}^{exact}(x, y, t) = \begin{bmatrix} \sin(\alpha_u \pi x) \cos(\alpha_u \pi y) \sin(t) \\ -\cos(\alpha_u \pi x) \sin(\alpha_u \pi y) \sin(t) \end{bmatrix},$$

$$p^{exact}(x, y, t) = \sin(\alpha_p \pi x) \sin(\beta_p \pi y) \sin(t),$$

$$c_i^{exact}(x, y, t) = \alpha_0 + \alpha_1 \cos(\alpha_c \pi x) \cos(\beta_c \pi y)\, e^{-\left(\alpha_c^2 + \beta_c^2\right) D \pi^2 t},$$

$$\phi^{exact}(x, y, t) = \gamma \log(c_i(x, y, t)),$$

Convergence Result

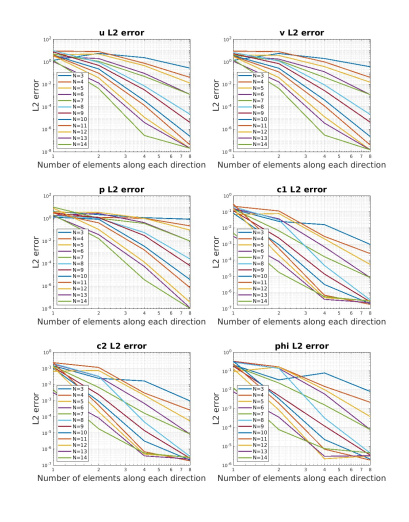

Figure 3: h convergence

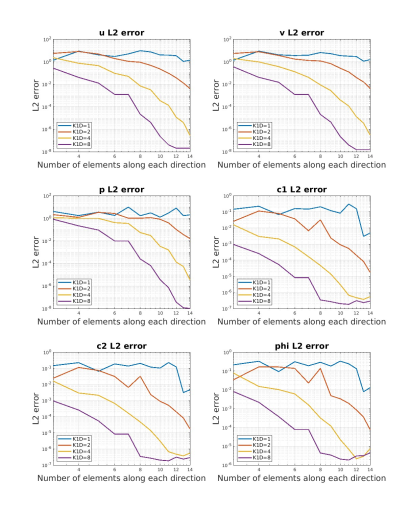

Figure 4: p convergence

Electrochemical reactions in turbulent flow

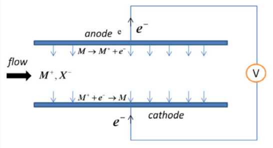

Figure 5: Test case setup[5]

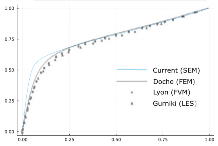

Figure 6: Mean concentration

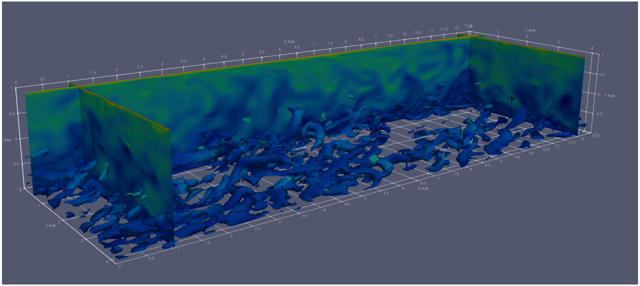

Figure 7: Mass transfer in channel flow with $Re_\tau = 180$, $Sc = 1$, $N = 7, 32 \times 8 \times 8$ elements

[5] Doche, F. Bauer, and Tardu, "Direct Numerical Simulation of an electrolyte deposition under a turbulent flow–A first approach"

In progress Work

- Convergence study of Butler-Volmer boundary condition

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- High Schmidt number simulations

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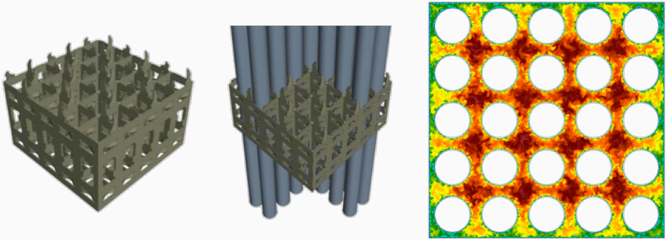

5x5 rod bundle mesh

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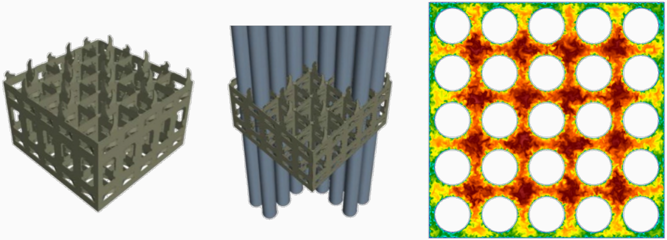

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- Stability and positivity preservation of PNP equations

Thank you!