Developing Spectral Element Methods for Molten Salt Reactors

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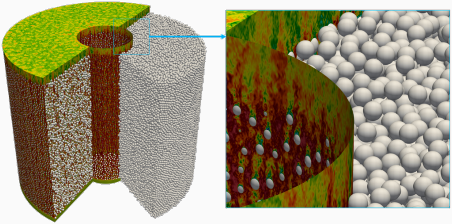
High Order Spectral Element Methods for PDEs

- Physical phenomena governed by PDE: nuclear reactors
- More accurate per degrees of freedom than low order methods (for smooth solutions)
- Nek5000/NekCEM/NekRS: scalable spectral element solver on CPU and GPGPU



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

Governing Equation

- Coupled system of incompressible Navier-Stokes and PNP equations

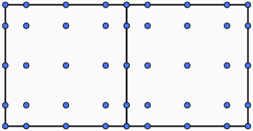
$$
\begin{aligned}
&\textit{Fluid}\begin{cases}
\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}\right)+\nabla p-\mu\nabla^2\boldsymbol{u} &= \nabla\cdot(\epsilon\nabla\phi)\,\nabla\phi+g\left(\frac{\rho_0-\rho(T)}{\rho_0}\right)\\
\nabla\cdot\boldsymbol{u} &= 0\\
\rho c_p\left(\frac{\partial T}{\partial t}+\boldsymbol{u}\cdot\nabla T\right) &= \nabla\cdot\left(\kappa\nabla T+\sum D_iQ_i\nabla c_i\right)
\end{cases}\\
&\textit{Ion}\begin{cases}
\frac{\partial c_i}{\partial t}+\nabla\cdot(\boldsymbol{N}_i+c_i\boldsymbol{u}) &= 0\\
\nabla\cdot\left(\sum z_i^2\mu_iFc_i\nabla\phi\right) &= \nabla\cdot\left[\sum z_i\left(c_i\boldsymbol{u}-D_i\nabla c_i-M_ic_i\nabla T\right)\right]
\end{cases}
\end{aligned}
$$

$$
\boldsymbol{N}_i=\underbrace{-D_i\nabla c_i}_{\text{diffusion}}\underbrace{-z_i\mu_iFc_i\nabla\phi}_{\text{migration}}\underbrace{-\frac{Q_iD_i}{RT^2}c_i\nabla T}_{\text{thermaldiffusion}}
$$

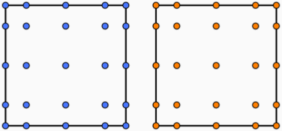
Numerical Discretization

- Discretization steps:
  - Step 1: Solve electroneutrality condition for electric potential ϕ^n
  - Step 2: Solve the ion transport equations for concentration $\mathbf{c}_i^n$
  - Step 3: Solve the incompressible Navier-Stokes equations with $\phi^n, \mathbf{c}_i^n$
- Temporal Discretization: BDF-k/EXT-k
- Spatial Discretization: Spectral element

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



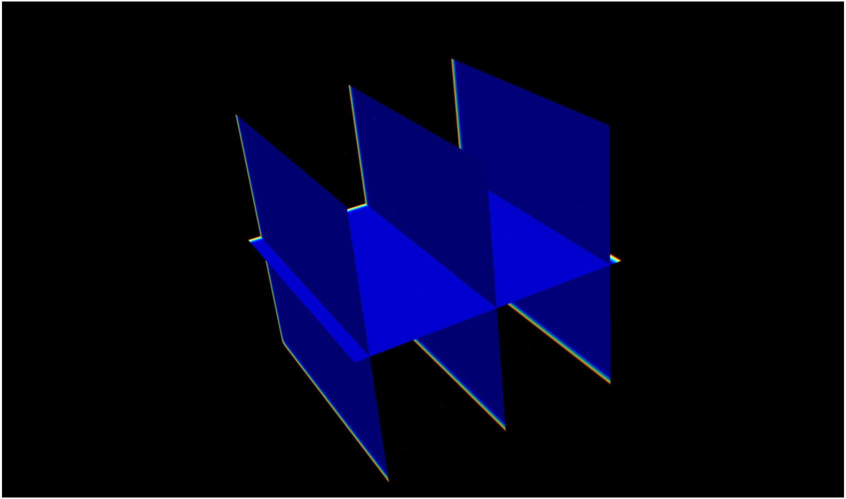
Global Representation



Local Representation

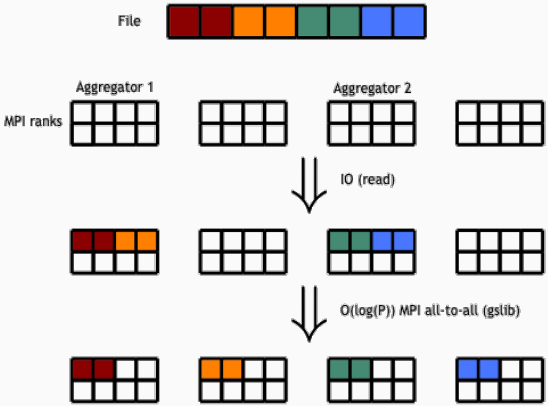
Numerical Results

- Verification on a box geometry



Parallel Read for Nek: ($P = 10^5 — 10^7$)

- Motivation: MPI I/O unavailable in some architectures (e.g. Fugaku)
- Simple MPI implementation for parallel read (collective buffering):

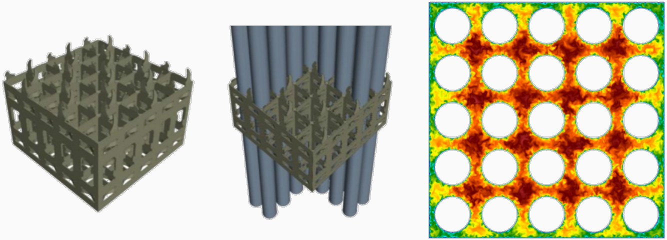


Future Work

- Electrode kinetics boundary conditions

$$\mathbf{N}_k \cdot \mathbf{n} = \begin{cases} 0 & \text{inert ion} \\ -\frac{i_n(c_k,\phi)}{z_k F} & \text{reactive ion} \end{cases}$$

- Run large scale simulations for molten salt reactor applications



5x5 rod bundle mesh

Thank you!