Westfälische
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Model Reduction of Microscale Li-Ion Battery Models

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The MULTIBAT Project

Gain better understanding of degradation processes in rechargeable Li-ion batteries through mathematical modelling and numerical simulation

- Focus on Li-plating, i.e. deposition of metallic Li at electrode/electrolyte interface.
- Funded by German Federal Ministry of Education and Research (BMBF).
- Participating institutes:

ulm university universität ulm — DLR Institute of Technical Thermodynamics — Fraunhofer ITWM — Applied Mathematics Münster

Associated industry partner: Deutsche ACCUmotive

Problem

- Li-plating is initiated at micrometre scale at interface between active electrode particles and electrolyte.
- Need microscale models which resolve active particle geometry.
- Result: huge non-linear discrete models.
  - Cannot be solved at cell scale on current hardware.
  - **Parameter studies extremely expensive, even on small domains.**

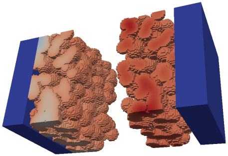

Figure : Simulation of microscale battery model on $48\mu m \times 24\mu m \times 24\mu m$ domain with random electrode geometry.

Microscale Model

- On each part of domain (electrode, electrolyte, current collector):

$$\frac{\partial c}{\partial t} - \nabla \cdot (\alpha(c,\phi)\nabla c + \beta(c,\phi)\nabla\phi) = 0 \qquad c : \text{Li}^+ \text{ concentration}$$

$$-\nabla \cdot (\gamma(c,\phi)\nabla c + \delta(c,\phi)\nabla\phi) = 0 \qquad \phi : \text{potential}$$

(α, β, γ, δ constant in first approximation)

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- Normal fluxes at particle/electrolyte interface are given by Butler-Volmer kinetics:

$$j_{se} = 2k\sqrt{c_e c_s (c_{max} - c_s)} \sinh\left(\frac{\phi_s - \phi_e - U_0(\frac{c_s}{c_{max}})}{2RT} \cdot F\right)$$
$$N_{se} = \frac{1}{F} \cdot j_{se}$$

Microscale Model

- Finite volume discretization with implicit Euler leads to

$$\begin{bmatrix} \frac{1}{\Delta t}(c_\mu^{(t+1)} - c_\mu^{(t)}) \\ 0 \end{bmatrix} + A_\mu\left(\begin{bmatrix} c_\mu^{(t+1)} \\ \phi_\mu^{(t+1)} \end{bmatrix}\right) = 0, \qquad c_\mu^{(t)}, \phi_\mu^{(t)} \in V_h$$

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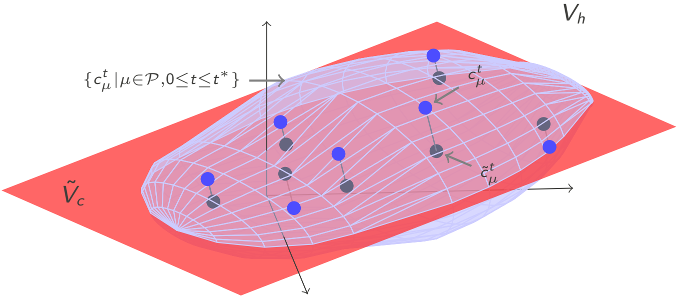
- $\mu \in \mathcal{P}$ indicates dependence on model parameters we want to vary (e.g. temperature T, charge rate).

The Reduced Basis Method

- Model order reduction technique for parameterized PDEs.
- Idea: Find solution in *problem adapted* low-dimensional reduced subspace of generic discrete function space.



The Reduced Basis Method

- **Online phase:** Determine reduced solution by solving projected equation

$$\begin{bmatrix} \frac{1}{\Delta t}(\tilde{c}_\mu^{(t+1)} - \tilde{c}_\mu^{(t)}) \\ 0 \end{bmatrix} + \{P_{\tilde{V}} \circ A_\mu\}\left(\begin{bmatrix} \tilde{c}_\mu^{(t+1)} \\ \tilde{\phi}_\mu^{(t+1)} \end{bmatrix}\right) = 0, \quad \tilde{c}_\mu^{(t)} \in \tilde{V}_c, \tilde{\phi}_\mu^{(t)} \in \tilde{V}_\phi$$

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- **Offline phase:** Build $\tilde{V}_c$, $\tilde{V}_\phi$ using iterative greedy algorithm:

function GREEDY($\mathcal{S}_{train} \subset \mathcal{P}$, ε, $\tilde{V}_c^0$, $\tilde{V}_\phi^0$)
  $\tilde{V}_c, \tilde{V}_\phi \leftarrow \tilde{V}_c^0, \tilde{V}_\phi^0$
  while $\max_{\mu \in \mathcal{S}_{train}}$ ERR-EST(RB-SOLVE(μ), μ) $> \varepsilon$ **do**
    $\mu^* \leftarrow \text{arg-max}_{\mu \in \mathcal{S}_{train}}$ ERR-EST(RB-SOLVE(μ), μ)
    $\tilde{V}_c, \tilde{V}_\phi \leftarrow$ BASIS-EXT($\tilde{V}_c$, $\tilde{V}_\phi$, SOLVE(μ^*))
  end while
  return $\tilde{V}_c, \tilde{V}_\phi$
end function

Empirical Interpolation

- Evaluation of

$$P_{\tilde{V}} \circ A_\mu : \tilde{V}_c \oplus \tilde{V}_\phi \longrightarrow V_h \oplus V_h \longrightarrow \tilde{V}_c \oplus \tilde{V}_\phi$$

still costly.

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- Use locality of finite volume operators: to evaluate M DOFs of $A_\mu(c, \phi)$ need only $M' \leq C \cdot M$ DOFs of (c, ϕ).

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$$P_{\tilde{V}} \circ A_\mu \approx P_{\tilde{V}} \circ (I_M \circ \tilde{A}_\mu \circ R_{M'})$$

where

$\tilde{A}_\mu$: A_μ restricted to M interpolation DOFs
I_M: Interpolation operator
$R_{M'}$: Restriction to M' DOFs needed for evaluation

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  - $\tilde{A}_\mu$: A_μ restricted to M interpolation DOFs
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  - $R_{M'}$: Restriction to M' DOFs needed for evaluation
- Use greedy algorithms to determine DOFs and interpolation basis.

Implementation

- Experimental implementation of battery model with Dune software framework.
- Model reduction with pyMOR.
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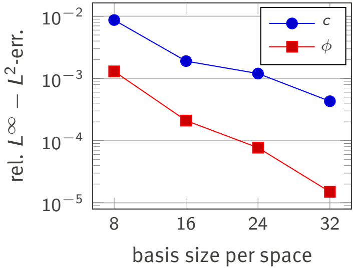
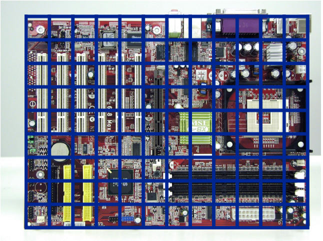
- Small 3D test case ($3.2 \cdot 10^4$ DOFs)
- $T \in [250,\ 350]\ K$
  $I_{charge} \in [10^{-4},\ 10^{-3}]\ A/cm^2$
- without operator interpolation
  ERR-EST = true error

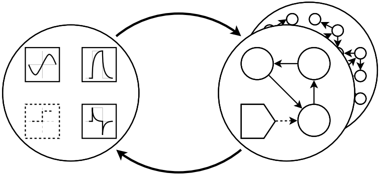


Other Applications

Localized Reduced Basis Methods for Maxwell's Equations



Model Reduction for Inverse Network Models



Thank you for your attention!

AG Ohlberger
`http://wwwmath.uni-muenster.de/num/ohlberger`

pyMOR – Model Order Reduction with Python
`http://pymor.org`

Model Reduction for Parameterized Systems
`http://morepas.org`