Model Reduction Approach to Battery Models

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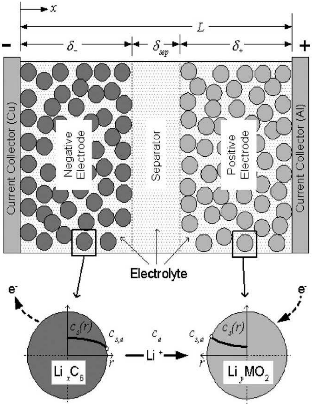
Outline of the talk

- Model equations and variational formulations
- Proper Orthogonal decomposition (POD) method
- POD Galerkin projection
- Other model reduction methods
- Questions and problems, and challanges

Lithium-ion battery



Model equations [Wu et al.]:

$$-\nabla\cdot(\kappa(c)\nabla\Phi_e) - S_e(\Phi_s - \Phi_e, c) = 0$$
$$-\nabla\cdot(\sigma\nabla\Phi_s) + S_e(\Phi_s - \Phi_e, c) + f = 0$$
$$(\varepsilon_e c)_t - \nabla\cdot\big(D\nabla c\big) = S_c(\Phi_s - \Phi_e, c)$$

$+$ Neumann boundary conditions

$$\int_\Omega \Phi_e \, \mathrm{d}\mathbf{x} = 0 \quad \text{(uniqueness)}$$

Varialbles:

electric potential Φ_e (electrolyte phase)
electric potential Φ_s (solid phase)
lithium ion concentration c (electrolyte)

Variational formulation

Weak solution

$$\int_\Omega \kappa(c)\nabla\Phi_e\cdot\nabla\varphi - S_e(\Phi_s-\Phi_e,c)\varphi\,\mathrm{d}\mathbf{x} = 0 \qquad \forall\varphi\in H^1(\Omega)$$

$$\int_{\Omega_s} \sigma\nabla\Phi_s\cdot\nabla\phi + \big(S_e(\Phi_s-\Phi_e,c)+f\big)\phi\,\mathrm{d}\mathbf{x} = 0 \qquad \forall\phi\in H^1(\Omega_s)$$

$$\int_\Omega (\varepsilon_e c)_t\chi + D\nabla c\cdot\nabla\chi - S_c(\Phi_s-\Phi_e,c)\chi\,\mathrm{d}\mathbf{x} = 0 \qquad \forall\chi\in H^1(\Omega)$$

Galerkin approximation

$\Phi_e(t,\cdot)\approx\sum_{i=1}^N\alpha_i(t)\varphi_i$, $\Phi_s(t,\cdot)\approx\sum_{i=1}^M\beta_i(t)\phi_i$, $c(t,\cdot)\approx\sum_{i=1}^L\gamma_i(t)\chi_i$
$\forall\varphi\in H^1(\Omega)\to$ for $\varphi_1,\dots,\varphi_N$, $\forall\phi\in H^1(\Omega_s)\to$ for $\phi_1,\dots,\phi_M$ etc.

Reduced-order model (ROM)

Use specific ansatz and test functions for your system.

Proper Orthogonal Decomposition (POD)

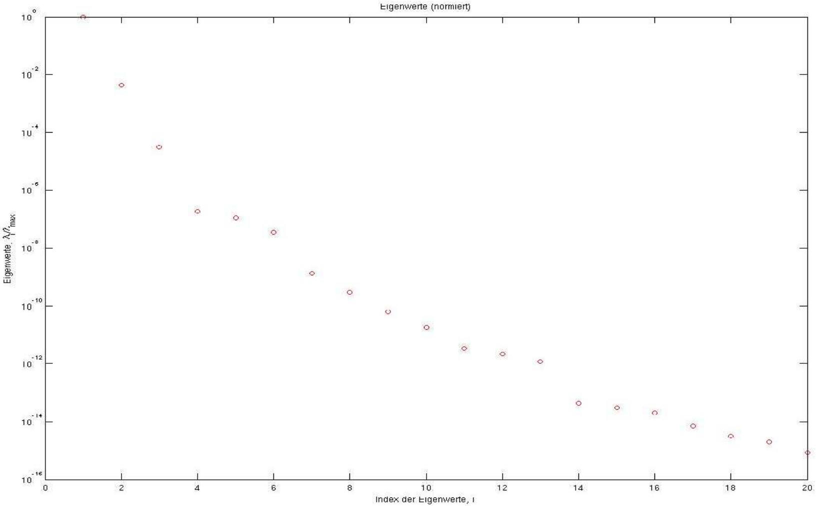
- Choose a time grid $0 \leq t_1 < \ldots < t_n \leq T$.
- Sample the snapshots $\{\Phi_e(t_j)\}_{j=1}^n$.
- Snapshot space $\mathcal{V}_e = \mathrm{span}\,\{\Phi_e(t_1), \ldots, \Phi_e(t_j)\}$
- Solve for $1 \leq \ell \leq n$ the minimization problem

$$\min_{\psi_1,\ldots,\psi_\ell} \sum_{j=1}^n \Big\| \Phi_e(t_j) - \sum_{i=1}^\ell \langle \Phi_e(t_j), \psi_i \rangle_X \, \psi_i \Big\|_X^2 \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle_X = \delta_{ij}$$

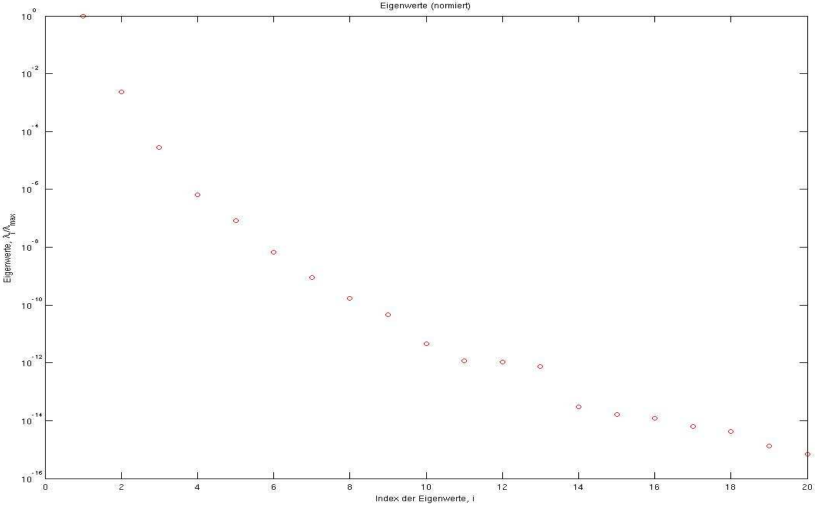
  with $X = L^2(\Omega)$ or $X = H^1(\Omega)$.

- Solution given by $\sum_{j=1}^n \langle \Phi_e(t_j), \psi_i \rangle_X \Phi_e(t_j) = \lambda_i \psi_i$, $1 \leq i \leq \ell$
- $\{\psi_i\}_{i=1}^\ell$ POD basis of rank ℓ.
- Analogous for the variables Φ_s and c.

Test with COMSOL [Ditz]: decay for the concentration c



Test with COMSOL [Ditz]: decay for the electric potential Φ_e (electrolyte phase)



ROM: POD Galerkin approximation

Ansatz:

$$\Phi_e(t) \approx \Phi_e^\ell(t) = \bar{\Phi}_e + \textstyle\sum_{i=1}^{\ell_1} \alpha_i(t)\psi_i^1, \qquad \bar{\Phi}_e \in H^1(\Omega)$$

$$\Phi_s(t) \approx \Phi_s^\ell(t) = \bar{\Phi}_s + \textstyle\sum_{i=1}^{\ell_2} \beta_i(t)\psi_i^2, \qquad \bar{\Phi}_s \in H^1(\Omega_s)$$

$$c(t) \approx c^\ell(t) = \bar{c} + \textstyle\sum_{i=1}^{\ell_3} \gamma_i(t)\psi_i^3, \qquad \bar{c} \in H^1(\Omega)$$

Weak solution

$$\int_\Omega \kappa(c)\nabla \Phi_e^\ell \cdot \nabla \psi_i^1 - S_e(\Phi_s^\ell - \Phi_e^\ell, c^\ell)\psi_i^1 \,\mathrm{d}\mathbf{x} = 0, \qquad 1 \le i \le \ell_1$$

$$\int_{\Omega_s} \sigma\nabla \Phi_s^\ell \cdot \nabla \psi_i^2 + \big(S_e(\Phi_s^\ell - \Phi_e^\ell, c^\ell) + f\big)\psi_i^2 \,\mathrm{d}\mathbf{x} = 0, \qquad 1 \le i \le \ell_2$$

$$\int_\Omega (\varepsilon_e c^\ell)_t \psi_i^3 + D\nabla c^\ell \cdot \nabla \psi_i^3 - S_c(\Phi_s^\ell - \Phi_e^\ell, c^\ell)\psi_i^3 \,\mathrm{d}\mathbf{x} = 0, \qquad 1 \le i \le \ell_3$$

Other model reduction methods

Classical methods for linear time-invariant systems

- Balanced truncation [Benner, Heinkenschloss, Sorensen,...]
- Moment matching [Bai, Freund, Gugercin,...]

Haves: a-priori error analysis for control problems

A further simulation-based method

- Reduced basis method [Maday, Ohlberger, Patera, Urban,...]

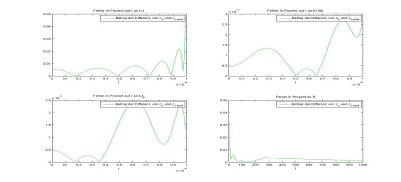
Haves: a-posteriori analysis for certain nonlinear PDES

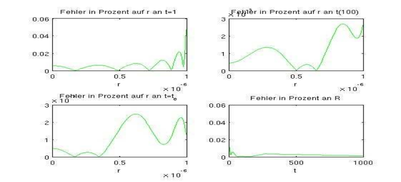
ROM as a surrogate model

Space mapping between fine (e.g., FE) model and coarse (ROM) model

Questions & Problems

Preliminary results





Questions and problems

- What is a efficient numerical method for the snapshot computation?
- How to choose the time grid (snapshot locations)?
- POD or reduced basis method?
- Can we estimate the errors $\|\Phi_e - \Phi_e^\ell\|$ etc.?
- Is ROM sufficiently accurate to estimate model parameters?