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Simulation Design Framework for Multiscale Multiphysics Thermo Electric and Electro Chemical Transport

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Outline

- Abstract
- Multiscale Multiphysics Simulation and Scientific Computing
- Simulation and Scientific Computing Changing Landscapes
- Phenomenological Equations Governing Transport Phenomena
- Linearized Boltzmann Transport Calculator for Thermoelectric Materials
- Dualfoil.py: Porous Electrochemistry for Rechargeable Batteries
- Frameworks Detail of Simulation Design for Multiscale Multiphysics Thermo Electric and Electro Chemical Transport
- Implementation Methodology
- Outlook
- References

ABSTRACT

nanoHUB btesolver and dualfoil resources enable studying thermo electric and electro chemical transport processes respectively. Simulation Design Framework for Optimizing the Multiscale Multiphysics Thermo Electric and Electro Chemical Transport in the respective devices is presented.

Multiscale Multiphysics Simulation and Scientific Computing

Simulation
Simulation helps in understanding, predicting and design of engineering systems based on its mathematical description that are governed by Fundamental and Phenomenological Laws following the multiscale, multiphysics and multidomain modelling paradigm
Scientific Computing
Scientific computing drives invention and discovery through the use of Simulation by Numerical Computation based on a Programming Algorithm using a Computational Hardware in the domains and disciplines of Energy, Biology, Computing, and Finance

Simulations using Multiscale, Multiphysics and Multidomain methodology is applicable in many chemical, physical, biological and additive manufacturing systems.

Simulation and Scientific Computing Changing Landscapes

Technology Used	*Paradigm Old*	*Paradigm Shift – Integration, Convergence, Synergy and Accessible*
Simulation	Physics driven	Data driven
Physics driven Simulation -	Computational Fluid Dynamics	Lattice Boltzmann Method

Multiscale Multiphysics Modeling		
Data driven Simulation	Ad Hoc Machine Learning I	Domain Specific Machine Learning II, Scientific Machine Learning
Machine Learning	Classical Machine Learning	Quantum Machine Learning
Accelerating Numerical Computations	CPU High Performance Computing	GPU, FPGA, ASIC, TPU, NPU, QPU High Performance Computing
Computing	Classical	Quantum, Biological, Analog, Reversible
HPC Resources	Centralized Cloud	Decentralized

		Blockchain
Simulation Data Interpretation Visualization	Off line	Real time
Software	Bare metal	Containerized, Virtualized, Cloud
Design Philosophy	Creative	Intelligent
Human Mobility	Drivered transport	Autonomous transport
Communication	Isolated	Connected
Research Funding	Central	Crowd
Scientific Inquiry	Top Down	Bottom Up
Programming Language	Compiled	Interpreted, Interpreted+Compiled
Operating System	Closed Sourced	Open Sourced

Licensing	Paid	Free
Algorithm Development	Corporate	Community
Innovation and Discovery	Adhoc Research	Academic Teaching/Learning Pedagogy
Reality	Physical	Virtual – VR, XR, MR, AR
Product Development	Experimental	Digital Twins
Curriculum development	Static and obsolete	Dynamic and futureready – Preempt the future, update pedagogy and includes Professional Development
Energy use	Online and interruptible	Stored and rechargeable

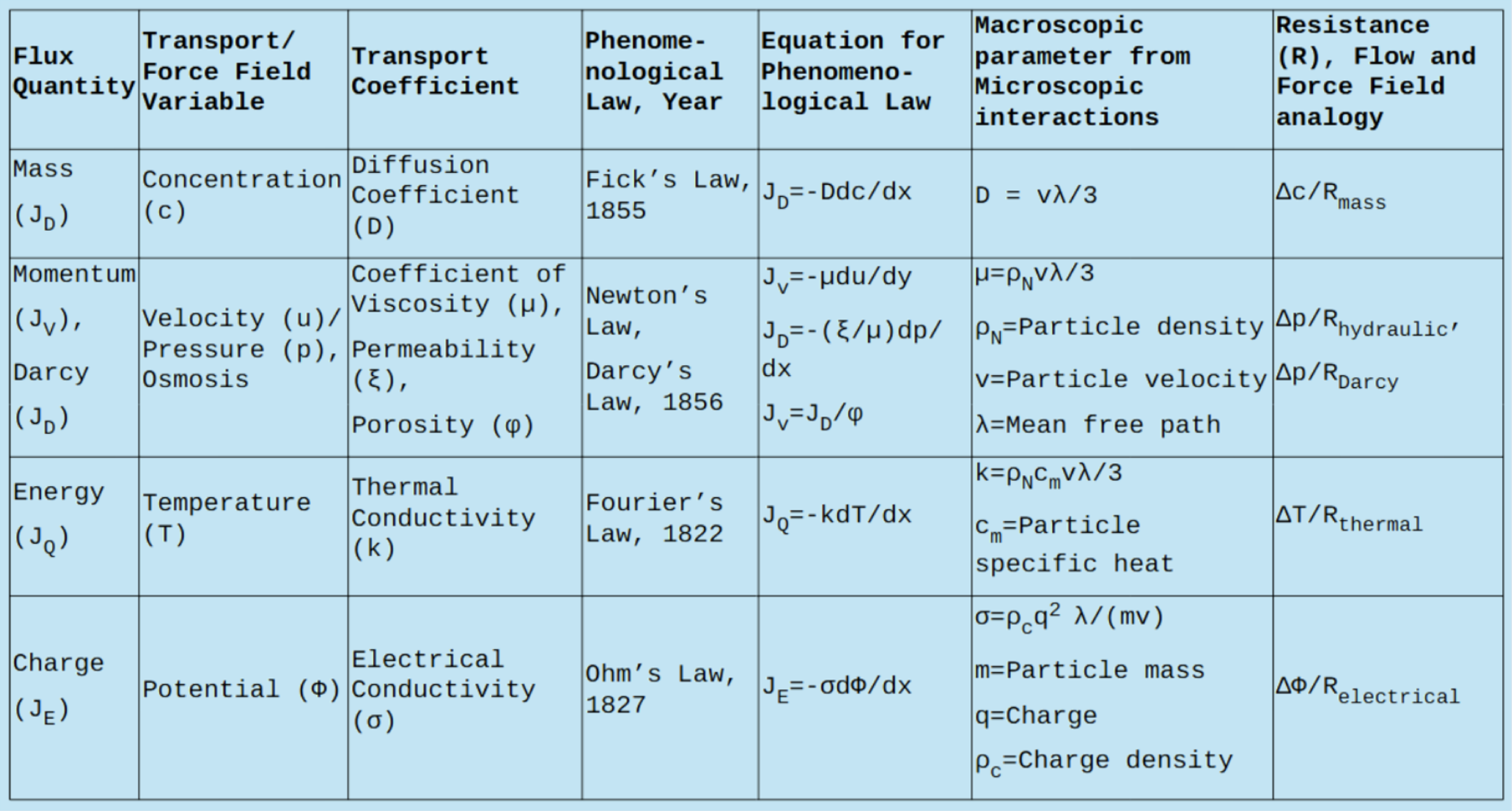
Energy generation	Fossil and polluting	Renewable and clean
Heterogeneous HPC Hardware	Fixed configuration and energy inefficient	Reconfigurable and energy efficient
Medicine	Curative Centralized	Preventive Point of Care
Electronic Design	Moore’s Law	Thermodynamic Limited
Computing Architecture	Incognitive	Neural Brain inspired
Entropy	Minimize disorder	Order from Disorder – Self organized
Programming Algorithms	Serial	Inherently parallel
Computer Memory	Separate	Unified

Industrial Revolution	Industry 1.0, 2.0, 3.0	Industry 4.0
Manufacturing	Substractive	Additive
Connected Devices	Consumer IoT	Industrial IoT
Data Analytics	Operational Forecasting	Strategic Innovation
Delivery Transport	Surface – Heavy Vehicle	Air – Portable Drone
High Performance Computing TFLOPS Workload	Off Line Cloud Computing	Real Time Edge Computing
Electronic Devices	Inorganic Semiconductor	Organic Semiconductor
Rechargeable Battery	Li-Ion	Li-Sulphur
Quantum Matter	3D Space	4D Space Time
Transport Phenomena	Classical Bulk	Quantum Topological

Hall Effect	Classical	Integer and Fractional Quantum
Complex System Self Organization	Classical Criticality	Quantum Criticality
Phase Transition	Classical	Quantum
Battery Technology	Classical Battery - Energy difference offered by electrochemical changes	Quantum Battery - Energy difference offered by different quantum states
Automotive Technology	Internal Combustion Engine Vehicle	Electric Vehicle
Quantum Fluid	4He	3He
Quantum Phenomena	Microscopic at Absolute Zero Kelvin	Macroscopic at Room Temperature

Design of Experiments	Physical Stochastic	Simulation Deterministic

Phenomenological Equations Governing Transport Phenomena



Flux Quantity	**Transport/ Force Field Variable**	**Transport Coefficient**	**Phenomenological Law, Year**	**Equation for Phenomenological Law**	**Macroscopic parameter from Microscopic interactions**	**Resistance (R), Flow and Force Field analogy**
Mass (J_D)	Concentration (c)	Diffusion Coefficient (D)	Fick's Law, 1855	$J_D=-Ddc/dx$	$D = v\lambda/3$	$\Delta c/R_{mass}$
Momentum (J_V), Darcy (J_D)	Velocity (u)/ Pressure (p), Osmosis	Coefficient of Viscosity (μ), Permeability (ξ), Porosity (φ)	Newton's Law, Darcy's Law, 1856	$J_V=-\mu du/dy$ $J_D=-(\xi/\mu)dp/dx$ $J_V=J_D/\varphi$	$\mu=\rho_N v\lambda/3$ ρ_N=Particle density v=Particle velocity λ=Mean free path	$\Delta p/R_{hydraulic}$, $\Delta p/R_{Darcy}$
Energy (J_Q)	Temperature (T)	Thermal Conductivity (k)	Fourier's Law, 1822	$J_Q=-kdT/dx$	$k=\rho_N c_m v\lambda/3$ c_m=Particle specific heat	$\Delta T/R_{thermal}$
Charge (J_E)	Potential (Φ)	Electrical Conductivity (σ)	Ohm's Law, 1827	$J_E=-\sigma d\Phi/dx$	$\sigma=\rho_c q^2\ \lambda/(mv)$ m=Particle mass q=Charge ρ_c=Charge density	$\Delta\Phi/R_{electrical}$

Linearized Boltzmann Transport Calculator for Thermoelectric Materials

nanoHUB btesolver is a Simulation tool to calculate thermoelectric transport properties such as Seebeck coefficient, electrical conductivity, and electronic thermal conductivity of bulk materials based on their multiple nonparabolic band structure information using the linearized Boltzmann transport equation under the relaxation time approximation. Estimation of thermoelectric properties for thermoelectric materials such as PbTe, Mg2SnSi and InGaAlAs can be performed using this simulation tools with possibility of adding new material library data.

Dualfoil.py: Porous Electrochemistry for Rechargeable Batteries

nanoHUB dualfoil.py allows to generate, organize, and visualize the electrochemical responses from various rechargeable battery systems with the ability to rapidly set up complex, multiscale simulations

Frameworks Details of Simulation Design for Multiscale Multiphysics Thermo Electric and Electro Chemical Transport

Complex systems simulations are very expensive and time consuming as they need high fidelity computing. Mathematical approximations such as Surrogate Modeling supplements simulations for analysis and optimization. In simulation experiments the experimental region is often too large having quantitative factors with many different levels. So as to maximize the information obtained within a minimum number of simulation runs, here we describe a simulation design framework based on DOE, to determine the factors that have the greatest influence on a response of the underlying system.

DOE is a systematic statistical method to study the relationship between multiple factors (independent variable) and responses (dependent variable) under investigation and used to optimize the process or phenomenon.

I One Factor at a Time Method

In a One Factor at a Time Method the value of one factor is changed, and then the response is measured. This process repeated with another factor.

II Full Factorial Method

In a Full Factorial Method all possible combinations of factor levels are used. Full factorial designs are represented by the form l^f, with l denoting the number of levels and f denoting the number of factors.

III Fractional Factorial Method

In a Fractional Factorial Method, a fraction of the number of design points of the corresponding full factorial is considered. The objective being to not waste design points for the estimation of effects that will almost certainly not be real.

IV Response Surface Method

Response Surface Method is used to model the curvature in the relationship between the factors and the response. It allows to find settings of factors to minimize or maximize a response.

V Taguchi Design Method

Taguchi Design Method is a type of general fractional factorial design. It is based on a design matrix proposed by Dr. Genichi Taguchi. A highly fractional orthogonal design allows to consider a selected subset of combinations of multiple factors at multiple levels.

VI Latin Hypercube Method

In a Latin hypercube design, the design points are spread uniformly throughout the experimental region. It is widely used in Simulation experimental designs as it covers the data space more evenly.

Implementation Methodology

Implementation methodology uses R language and environment for statistical computing that supports Design of Experiments (DoE) and Analysis of Experimental Data.

Sample Methodology for Full Factorial Method

```
library(DoE.base)
```

```r
design <- fac.design(nlevels=3, nfactors=3, factor.names =
list(x1=c(-1,0,1), x2=c(-1,0,1), x3=c(-1,0,1)), randomize=FALSE)
design
```

```
   x1 x2 x3
1  -1 -1 -1
2   0 -1 -1
3   1 -1 -1
4  -1  0 -1
5   0  0 -1
6   1  0 -1
7  -1  1 -1
8   0  1 -1
9   1  1 -1
10 -1 -1  0
11  0 -1  0
12  1 -1  0
13 -1  0  0
```

14	0	0	0
15	1	0	0
16	-1	1	0
17	0	1	0
18	1	1	0
19	-1	-1	1
20	0	-1	1
21	1	-1	1
22	-1	0	1
23	0	0	1
24	1	0	1
25	-1	1	1
26	0	1	1
27	1	1	1

For estimating the interaction effects the analyses is performed using coded values of factors

Sample Methodology for Response Surface Method

```
library(rsm)
design <- bbd(3, randomize=FALSE)
design
```

```
     x1  x2  x3
1    -1  -1  0
2    1   -1  0
3    -1  1   0
4    1   1   0
5    -1  0   -1
6    1   0   -1
7    -1  0   1
8    1   0   1
9    0   -1  -1
10   0   1   -1
11   0   -1  1
12   0   1   1
13   0   0   0
14   0   0   0
```

15	0	0	0
16	0	0	0

To determine the optimum operating conditions for the system or to determine a region of the factor space in which operating requirements are satisfied the curvature of the response surface is explored by using a quadratic regression equation.

Outlook

1) Using Machine Learning Linear and Non-Linear Models in Response Surface Method
2) Integrating Experimental Designs with Digital Twins
3) Using Metaheuristic Optimization algorithms in Latin Hypercube Method

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