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Multiscale Multiphysics Modeling Framework for Industry 4.0

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ABSTRACT Many of the traditional learning methods cannot be applied with

competency foundations for Industry 4.0 expertise. Industry 4.0 Competency is based on Multiscale Multiphysics (MSMP) Modeling Foundation similar with that of Scientific Machine Learning link to Domain Specific Foundations. Multiscale Multiphysics modeling considers simultaneously at different scales coupled physics that benefit from combining both macroscopic as well microscopic models. Macro, micro-nano and quantum scale modeling governing multiphysical phenomena is brought under a common umbrella of Scientific Computing framework for the Inter/Multi disciplinary and domains of Energy, Biology, Computing and Finance, as outlined in this presentation. Digital Twin concept entailing integrated Multiscale Multiphysics simulations will play a decisive role towards successful Industry 4.0 deployment and acceptance.

Simulation and Scientific Computing

Simulation Scientific Computing 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 and multiphysics modelling paradigm

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

Why Simulation

Simulation is driving Scientific and Engineering Innovation Innovation is key to Organization, Institution, Industry and Individual Success Innovation results in optimizing Engineering Design Manufacture of products under economic and time constraints

MSMP Modeling Framework

- ➢ Multiscale modeling enables understanding of the physics governing the phenomena under study and provides insights to the interplay and drivers of coupled processes at the overlapping time and spatial scales

- ➢ Macro, micro-nano and quantum scale modeling
governing multiphysical phenomena is brought under a common umbrella of Scientific Computing framework for the Inter/Multi disciplinary and domains of Energy, Biology,

Computing and Finance, as outlined below

Richard Multiscale
Feynman's comments Multiphysics
related to Modeling Framework Modeling
Framework Course
Governing Equations

Computational Fluid Dynamics/ Mechanics
'Turbulence is the most important unsolved problem of classical physics'
Navier Stokes Equation/Finite Difference Equation
MEMS & Micro- Nano Fluidics

'There's Plenty of Room at the Bottom'
Boltzmann Transport Equation/ Lattice Boltzmann Equation Non-Equilibrium & Quantum Thermodynamics

'One quantum system might be used to

efficiently simulate the dynamics of other

quantum system of interest - the Universal

Quantum Computer’
Schrodinder Equation/Lindblad Quantum Master Equation

Technology Futureproof [3]

Technology Reference Publication

Simulation Training guide on

computer aided engineering and

design,

http://www.engineersjournal.ie/2015/10/27/training-guide-on-computer-aided-

engineering-and-design/, 2015. Energy Role of Mechanical Engineering in Modern Biology and Medicine, http://www.engineersjournal.ie/2018/01/09/mechanical-engineering-modern-biology - medicine/, 2018. Quantum Mechanical engineering must futureproof to maximize tomorrow’s technology, http://www.engineersjournal.ie/2017/06/06/mechanical-engineering-futureproof-tomorrows-technology/, 2017

M SMP Modeling Framework Scope [1]

Computational Fluid Dynamics/Mechanics

Scope: Numerical treatment of the physics of fluid flows incorporating energy, species and momentum transport mechanisms. Understanding of fundamental concepts through review of governing equations, numerical discretisation of finite difference, finite volume and finite elements methods covering the types of fluids flows namely incompressible, compressible, laminar and turbulence, newtonian and complex fluids. In CFD study the simulation is carried at macro scales. Good grasp of continuum based simulation tools is needed for numerical maths handling using FDM, OpenFOAM based on FVM and Elemer based on FEM.

MEMS & Micro-Nano Fluidics

Scope: Physics at Micro, Nano and Molecular scales manipulating very small volumes of fluid with handling of new phenomena. Fluid flows incorporating energy, species and momentum as well as charge transport mechanisms are covered.
Understanding through fundamental concepts of surface tension driven capillary, electrokinetic and slip flow

phenomena are important. In MEMS & Micro-Nano Fluidics study the simulation is carried at micro-nano or atomic/molecular scales. Methods for simulation available are, particle based Molecular dynamic, Direct Simulation Monte Carlo, Lattice Boltzmann Method, Boltzmann Transport Equation with emphasis on Multiphysics and Multiscale modeling approaches.

Non-Equilibrium & Quantum Thermodynamics [4]

Scope: Unified understanding of complex systems such as quantum energy transport, computing, biology and finance. Understanding of fundamental concepts of kinetic gas theory, Statistical Thermodynamics, Non-equilibrium or Irreversible thermodynamics, Quantum mechanics are included here. Irreversible process and coupled phenomena can be studied. In Non-Equilibrium & Quantum Thermodynamics study the simulation is carried encompassing all the above mentioned scales ie. multiscale modeling including sub atomic quantum scales. Available tools for exploring Quantum simulation are ShengBTE and QuTiP.

Industry 4.0 Enablers and Paradigm Shift in Technology

Use in Current Times [2, 4]

Technology Enabler Used and Paradigm Old

Paradigm Integration, Synergy and Shift

Convergence, Accessible – Simulation Physics driven Data driven Physics driven Simulation -

Multiscale Multiphysics Modeling
Computational Fluid Lattice Boltzmann Method

Dynamics Data driven Simulation Ad Hoc Machine

Learning I Domain Specific Machine Learning II,

Scientific Machine Learning Machine Learning

Classical Machine Quantum Machine Learning

Learning Accelerating Numerical CPU High
Performance GPU, FPGA, ASIC, TPU, NPU,

Computations Computing 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 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 Learning
Classroom Online Operating System Closed Sourced Open Sourced Licensing Paid Free Algorithm Development Corporate Community Skill Sets Discipline specific Multi talented Journal Publication Subscription Open
Innovation and Discovery Adhoc Research

Academic Teaching/Learning Pedagogy Event Live

Remote, VR Reality Physical Virtual Product Development Experimental Digital Twins Lectures Seminar Webinar Recruitment In Campus Off Campus Experience Real Portfolio Business Profit endeavour and disruptive Social responsible and inclusive Curriculum development Static and obsolete Dynamic and futureready – Preempt the future, update pedagogy and includes Professional Development Training Rigid and inflexible Adaptable and seamless transition Energy use Online and interruptible Stored and rechargeable Energy generation Fossil and polluting Renewable and clean

Heterogenous HPC Hardware Fixed configuration and energy inefficient Reconfigurable and energy efficient Job functions Predefined Evolves with time

and flexible 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 Workplace Corporate Office Remote Working Connected Devices Consumer IoT Industrial IoT Professional Skill Sets Remain Competitive Future

Ready and Future Proof Data Analytics Operational

Forecasting Strategic Innovation
Delivery Transport Surface – Heavy Vehicle Air –

Portable Drone High Performance Computing

TFLOPS Workload
Off Line Cloud Real Time Edge Computing

Computing Electronic Devices Inorganic

Semiconductor Organic Semiconductor High

performance light harvesting organic semiconductor

solar cells

Maximize the area of the interface between the

electrodes and the organic semiconductors

Minimize the area of the interface between the

electrodes and the organic semiconductors

M SMP Modeling in Industry 4.0 [2]

➢ Digital Twin is the basic enabling technology of
Industrial 4.0

➢ Digital Twin uses virtual model, sensors data and historical past data for real time decision making

➢ For a successful Digital Twin concept, it needs to integrate Multiscale and Multiphysics simulation technology to provide real-time predictions of system behavior

MSMP Modeling Insight to Medical treatment of

Diseases [2]

➢ Computational Fluid Dynamics/Mechanics – Diagnostics of Disease

➢ MEMS & Micro-Nano Fluidics – Drug Delivery

➢ Non-Equilibrium & Quantum Thermodynamics – Molecular Understanding of Drug and its effect on Disease

R ole of Topology in Multiscale Multiphysics

Modeling [2]

Non-Equilibrium & Quantum Thermodynamics

Fractional Quantum Hall effect – Topology Quantum Phenomena

MEMS and Micro- Nano Fluidics

Anisotropic liquid crystal complex fluid flow – Topology Microfluidics

Computational Fluid Mechanics/Dynamics

Optimality Criteria based Topology Optimization

R eferences

[1] Auro Ashish Saha, 2017, Mechanical

engineering must futureproof to maximise

tomorrow's technology,

http://www.engineersjournal.ie/
2017/06/06/mechanical-engineering-futurep
roof-tomorrows- technology/

[2] Auro Ashish Saha, Skills for Industry 4.0, Summer Vacation Specific Field Knowledge Training: Professional Development Course PDC02, Pondicherry Engineering College, Pondicherry, 2020.

[3] Auro Ashish Saha, Super Quantum Engineer (AGNIi #5290), 02-09- 2019.

[4] Auro Ashish Saha, 2019, Non-equilibrium and Quantum

Thermodynamics, MEP30. B.Tech.

(Mechanical) – VII Semester, Lecture Notes, Pondicherry Engineering College, Pondicherry