Learning Everywhere Resource for BDEC

Compiled by Geoffrey Fox, Updated July 27, 2019

General Links

A. BDEC Home Page and set of workshops [1], [2]
B. First BDEC meeting at Bloomington with full links including videos [3]
C. BDEC Bloomington meeting Application Working Group
D. Darpa components of a good demonstrator.
E. MLPerf Consortium [4]
    a. MLPerf HPC working group and datasets
    b. MLPerf Deep Time Series working group and Collection of Datasets

Learning Everywhere Projects

A. **Deep Learning to Control Plasma Fusion** (Bill Tang, Princeton)
    a. One slide banner
    b. Paper published in Nature [5]
    c. DoE News Release [6]
    d. The associated Fusion RNN AI/DL predictive code is open source with a GitHub link specified in the paper; and
    e. The Gyrokinetic Toroidal Code (GTC) is the exascale-capable fully electromagnetic direct numerical simulation (DNS) particle-in-cell (PIC) code that will be used to help develop reduced models of pre-disruption classifiers. (http://phoenix.ps.uci.edu/GTC/).
    f. BDEC Presentation on deep learning for fusion [7]

Learning Everywhere Links

General Discussions

1. Initial Poznan Manifesto for learning everywhere
2. Jeffrey Dean presentation at NIPS 2017 on Machine learning for systems and systems for machine learning [8]
3. Microsoft 2018 Faculty Summit presentations on AI for Systems [9], [10]
4. Satoshi Matsuoka on the convergence of AI and HPC [11]
5. An NSF funded project mainly focused on HPCforML [12], [13]
6. Learning Everywhere papers commenting on Technology, Network Science, nanoengineering, biomolecular and computational biology (virtual tissues) with a short published paper [14] and longer report [15] plus a presentation at BDEC [16] and at IPDPS [17].
7. A broad discussion of machine learning for climate change. [18]

Computer Science Issues

8. Papers on Uncertainty Quantification with Machine Learning [19]–[23]
9. Paper on learning index structures for search with machine learning [24]
10. Paper [25] on how to scale CNN's as problems scale.

11. Paper using ODE's to build a continuous neural network rather than one built from a set of layers [26] with a recent theoretical analysis [27]

Categories used below to categorize papers [14]–[16], [28]

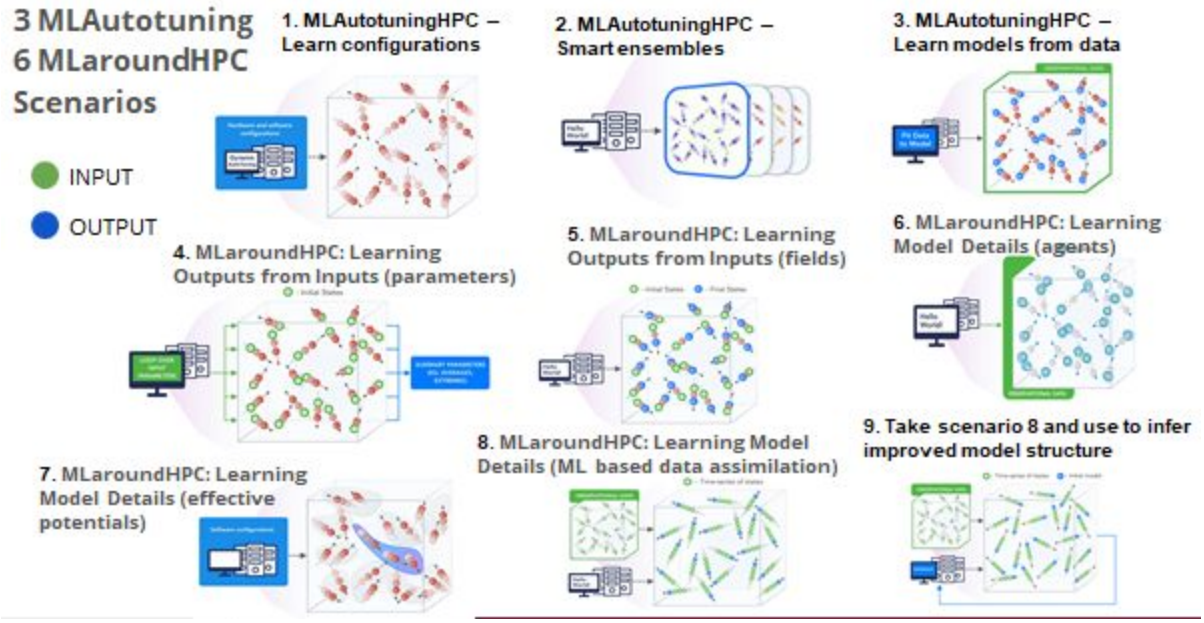
- **HPCforML:** Using HPC to execute and enhance ML performance, or using HPC simulations to train ML algorithms (theory guided machine learning), which are then used to understand experimental data or simulations.
- **MLforHPC:** Using ML to enhance HPC applications and systems

We further subdivide **HPCforML** as

- **HPCrunsML:** Using HPC to execute ML with high performance
- **SimulationTrainedML:** Using HPC simulations to train ML algorithms, which are then used to understand experimental data or simulations.

We also subdivide **MLforHPC** as

- **MLAutotuning:** Using ML to configure (autotune) ML or HPC simulations.
- **MLafterHPC**: ML analyzing results of HPC as in trajectory analysis and structure identification in biomolecular simulations
- **MLaroundHPC:** Using ML to learn from simulations and produce learned surrogates for the simulations. The same ML wrapper can also learn configurations as well as results. This differs from SimulationTrainedML as the latter is typically using learned network to predict observation whereas in MLaroundHPC we are using the ML to improve the HPC performance. The figure specifies 9 subcategories in the MLAutotuning and MLaroundHPC spaces.
- **MLControl:** Using simulations (with HPC) in control of experiments and in objective driven computational campaigns. Here the simulation surrogates are very valuable to allow real-time predictions.



Experiment Control

12. *MLControl:* Controlling Tokomaks using data and simulation to predict instabilities [5]–[7]
13. *MLControl:* Use of machine learning in experiment control [29]
14. *MLControl:* Use of deep learning in control of material science experiments at light sources [30]

General Simulations-MLAutotuningHPC – Smart ensembles

15. *MLAutotuningHPC – Smart ensembles:* Use of visualization to control smart ensembles of simulation [31]

Particle Dynamics Simulations

Particle Dynamics-Review

16. MLandHPC (review): Use of Machine Learning to enhance biomolecular simulations [32]; review of different MLandHPC patterns of interest in biomolecular simulations.
17. MLandHPC (review): NIPS 2018 Workshop on machine learning in material science and molecular dynamics [33] with some but not all papers available. There is a follow-up book [34]
18. MLforHPC: Review of simulation and some machine learning methods (not emphasized) used in macromolecular structure and dynamics [35]

Particle Dynamics-MLAutotuningHPC – Learn configurations

19. Nanoparticle simulations using *MLAutotuningHPC – Learn configurations* to improve performance [36] and *MLaroundHPC: Learning Outputs from Inputs (parameters)* [37] defining surrogates learnt as a function of defining parameters

Particle Dynamics-MLAutotuningHPC – Smart ensembles

20. *MLAutotuningHPC – Smart ensembles:* Review of techniques for smart ensembles [38]
21. *MLAutotuningHPC – Smart ensembles:* Use of machine learning to guide molecular dynamics simulations to explore full range of phase space [39]. Manifold learning is used to find a low dimension set of collective variables and then to learn dynamics in those variables.
22. *MLAutotuningHPC – Smart ensembles:* Use of Machine Learning (Best Arm Identification method) to optimize determination of protein-ligand binding (docking) energies when total compute resources are constrained, [40]
23. *MLAutotuningHPC – Smart ensembles:* Efficient exploration of configuration space by adding an adaptively computed biasing potential using machine learning to the original dynamics. [41]–[44]
24. *MLAutotuningHPC – Smart ensembles:* Loop over multiple molecular dynamics and Deep Learning steps to more accurately sample phase for long time computations - termed “Reweighted autoencoded variational Bayes for enhanced sampling (RAVE)” [45], [46]

Particle Dynamics-MLaroundHPC: Learning Outputs from Inputs (parameters)

25. *MLaroundHPC: Learning Outputs from Inputs (parameters):* An early paper in 2012 using non-ANN machine learning to learn energies from molecular properties [47]
26. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Use of DNN to learn crystal energies and stability with training data calculated by DFT. [48]
27. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Review of machine learning (emphasized) for molecular and materials science [49]
28. Nanoparticle simulations using *MLAutotuningHPC – Learn configurations* to improve performance [36] and *MLaroundHPC: Learning Outputs from Inputs (parameters)* [37] defining surrogates learnt as a function of defining parameters
29. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Review article on machine learning to predict material properties from structure of compounds. Uses observation and simulations to determine structure-property relationships for training [50]
30. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Use of neural nets to describe potentials and simulation results for Infrared Spectra [51] The input features to the ANN's are the parameters of Frenkel exciton Hamiltonians and the output average exciton transfer times and overall transfer efficiencies.
31. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Machine Learning (kernel ridge regression) to map database (of DFT simulations) into material properties. [52]
32. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Machine Learning (kernel ridge regression) to map database (of DFT simulations) into valence charge densities. [53], [54]
33. *MLaroundHPC: Learning Outputs from Inputs (parameters):* ANN's for fast estimate of excitation energy transfer properties (used in solar cells) [55]. The ANN is used to map Hamiltonian specifications into material properties.
34. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Machine Learning to predict the energies and forces and avoid repetitive computations [56]. A decision engine decides whether to use learnt result or calculate using full simulation.
35. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Machine Learning used to estimate forces in molecular simulations choosing between ab initio Quantum mechanics or regression based ML estimate from a database enhanced dynamically. [42], [57]
36. *MLaroundHPC: Learning Outputs from Inputs (fields):* Investigation of different neural network structures to learn the results of an Ising model simulation near its critical point comparing with classic Monte Carlo using a combination of single-site Metropolis and Wolff cluster updates [58]
37. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Review of machine learning with dimensionality reduction and clustering algorithms, drug discovery DeepTox, free-energy surface of molecules, ligand binding site detection, ligand pose prediction, ligand, active/inactive classification, ligand binding affinity prediction, and protein design, DeepChem software, MoleculeNet challenge and access to relevant QSAR prediction datasets. Two cases covered in detail - ML representation of Quantum forces and prediction of binding affinities. [59]
38. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Deep Learning to study compositional and configurational chemical space for molecules of intermediate size. Focus on use of a particular representation of input molecular structure [60].
39. *MLaroundHPC: Learning Outputs from Inputs (parameters):* Specifying atom representations for input into machine learning [61]

40. *MLaroundHPC: Learning Outputs from Inputs (parameters)* is reviewed but generalized to learn system wavefunction in its hamiltonian matrix element form allowing richer set of predictions with *MLaroundHPC: Learning Outputs from Inputs (fields)* [62]

Particle Dynamics-MLaroundHPC: Learning Outputs from Inputs (fields)

41. *MLaroundHPC: Learning Outputs from Inputs (fields):* An early paper using in 1994 neural nets to solve ODE's. [63]
42. *MLaroundHPC: Learning Outputs from Inputs (fields):* Investigation of different neural network structures to learn the results of an Ising model simulation near its critical point comparing with classic Monte Carlo using a combination of single-site Metropolis and Wolff cluster updates [58]
43. *MLaroundHPC: Learning Outputs from Inputs (parameters)* is reviewed but generalized to learn system wavefunction in its hamiltonian matrix element form allowing richer set of predictions with *MLaroundHPC: Learning Outputs from Inputs (fields)* [62]
44. *MLaroundHPC: Learning Outputs from Inputs (fields):* Using Generative Adversarial Networks to produce surrogates of large scale simulations of the effect of gravitational lensing used to study early universe CosmoGAN [64], [65] with supplement [66] on Github

Particle Dynamics-MLaroundHPC: Learning Model Details (effective potentials)

45. *MLaroundHPC: Learning Model Details (effective potentials):* Use of machine learning to generate an effective Hamiltonian using initial local updates as training data to choose correlated update spins with Wolff's method near a critical point [67]. This is applied in [68]
46. *MLaroundHPC: Learning Model Details (effective potentials):* Neural-network representation [69]–[72] of DFT potential-energy surfaces
47. *MLaroundHPC: Learning Model Details (effective potentials):* MLaroundHPC: General framework for calculating a many-body coarse-grained potential. [73]
48. *MLaroundHPC: Learning Model Details (effective potentials):* Formulate coarse-graining as a supervised machine learning problem and use coarse-graining error and cross-validation to select and compare the performance of different models. [74]
49. *MLaroundHPC: Learning Model Details (effective potentials):* Review of the use of neural networks to represent potentials and speed up simulations [75]. Has plot of physics, chemistry and materials papers per year using ANN's. There are 1500 per year after 2010.

Particle Dynamics-MLaroundHPC: Learning Model Details (coarse graining)

50. *MLaroundHPC: Learning Model Details (coarse graining):* VAMP(variational approach for Markov processes)nets to learn end to end reduced complexity surrogates of molecular dynamics without custom modelling such as transformation of simulated coordinates into structural features, dimension reduction, clustering the dimension-reduced data, and estimation of a Markov state models [76]
51. *MLaroundHPC: Learning Model Details (coarse graining):* Use of collective variables (dimension reduction) to study protein dynamics [77]

52. *MLAutotuningHPC – Smart ensembles, MLaroundHPC - Learning Model Details (coarse graining):* Collective variables to sample molecular dynamics and free energy landscape [78]–[80]
53. *MLAutotuningHPC – Smart ensembles, MLaroundHPC - Learning Model Details (coarse graining):* Use of machine learning to support long time scale molecular simulations [81] Reviews other approaches such as RAVE and VAMP.

Particle Dynamics-MLaroundHPC: Learning Model Details (agents)

54. *MLaroundHPC: Learning Model Details (agents)* Use of ANN's to represent dynamics of robots [82]

Particle Dynamics-MLafterHPC

55. *MLafterHPC:* Software packages for analyzing results of molecular dynamics simulations MDAnalysis [83], [84] and CPPTraj [85], [86]
56. *MLafterHPC:* Machine learning to identify crystal structure from molecular dynamics simulations [87]
57. *MLafterHPC:* Machine learning (SVM) to analyze structure produced in simulated glassy systems [88]
58. *MLafterHPC:* Machine Learning to classify phases of quantum Monte Carlo simulations of the Hubbard model [89]
59. *MLafterHPC:* Machine Learning used in materials simulation to aid the design of new materials and to understand properties [90]–[96]
60. *MLafterHPC:* Use of Graph Networks to improve prediction of properties of Molecules and Crystals. [97]
61. *MLafterHPC:* Using machine learning to analyze results of cosmology simulations to determine parameters of the universe [98] and implemented with Cosmoflow Deep Learning framework [99]
62. *MLafterHPC:* Data-mining and manifold learning techniques to detect the slowly varying components of dynamical systems [60]
63. *MLafterHPC:* Machine Learning for a systematic approach to reduce the dimensionality of a complex molecular system [100]. Uses decision trees (XGBoost) and dimension reduction (PCA).

Agent-Based Simulations and Data-driven Approaches to ABM systems

ABM-HPCforML-SimulationTrainedML

64. *HPCforML-SimulationTrainedML*: Using models to fill in gaps in bioinformatics data [101]

ABM-MLAutotuningHPC – Smart ensemble

65. *MLAutotuningHPC – Smart ensembles:* Smart ensembles for cancer agent based models with PhysiCell. [102]

ABM-MLAutotuningHPC – Learn models from data

66. *MLAutotuningHPC – Learn models from data:* Machine-learning (XGBoost) and intelligent sampling to build a surrogate meta-model to calibrate agent-based models with data [103]

67. *MLAutotuningHPC – Learn models from data*: Using machine learning (modest emphasis) to represent cell (agent) behavior based on data for prediction of cancer cell behavior [104]
68. *MLAutotuningHPC – Learn models from data*: Automatic inference of a model of the escape response behavior in a roundworm directly from time series data [105] building on [106], [107]. The unknown parameters in a set of ODE's are determined by fitting data in a hierarchical fashion.

ABM-MLaroundHPC: Learning Outputs from Inputs (fields)

69. *MLaroundHPC: Learning Outputs from Inputs (fields):* Use of Deep Learning LSTM to produce surrogates of a one-dimensional biological agent simulation [108] with paper and supplement.
70. *MLaroundHPC: Learning Outputs from Inputs (fields):* Deep Learning for Agent-based Epidemic Forecasting DEFSI with ANN's learning detailed (county level) information from simulations. [109]

ABM-MLaroundHPC: Learning Model Details (ML based data assimilation)

71. *MLaroundHPC: Learning Model Details (ML based data assimilation):* Using data to predict solutions of complex coupled Agents for metabolic pathway dynamics [110]
72. *MLaroundHPC: Learning Model Details (ML based data assimilation):* Deep Learning RNN and CNN to predict epidemics viewed as time series [111]
73. *MLaroundHPC: Learning Model Details (ML based data assimilation):* LSTM Flu epidemic forecasting enhanced by environmental data such as climate [112]

Partial Differential Equation Based Simulations

PDE-MLaroundHPC - Learning Outputs from Inputs (parameters)

74. *MLaroundHPC - Learning Outputs from Inputs (parameters):* Finding coefficients of a PDE that reproduce observed data [113]
75. *MLaroundHPC - Learning Outputs from Inputs (parameters):* Machine Learning surrogates of heart simulations to speed up aortic aneurysm studies [114]

PDE-MLaroundHPC: Learning Outputs from Inputs (fields)

76. *MLaroundHPC: Learning Outputs from Inputs (fields):* Finding forward (direct) and inverse mapping functions of input to output. The inverse map is particularly interesting as it is no harder than direct method for ANN's but classic PDE solvers only give direct map straightforwardly. [115], [116]
77. *MLaroundHPC: Learning Outputs from Inputs (fields):* Deep Learning for solving partial differential equations [117], [118] (called Physics Informed Neural Net PINN) extended to nonlinear systems [119]
78. *MLaroundHPC: Learning Outputs from Inputs (fields):* Uses PINN to solve stochastic forward and inverse problems with separate DNN to learn error. [120]
79. *MLaroundHPC: Learning Outputs from Inputs (fields):* Deep learning to find surrogates for fluid flow simulations [121]
80. *MLaroundHPC: Learning Outputs from Inputs (fields):* Use of machine learning to improve Extended dynamic mode decomposition for representing Koopman Operator to

represent dynamical systems. The ANN learns the operators used to represent the solution.[122]

81. *MLaroundHPC: Learning Outputs from Inputs (fields):* Solving high dimensional (up to 1000's) partial differential equations using deep learning surrogates with differentiation of neural net form and no mesh points. Exact solutions used to train surrogates [123], [124]
82. *MLaroundHPC: Learning Outputs from Inputs (fields):* Explicitly differentiating the ANN in [114] solving advection and diffusion type PDEs in complex geometries[125]

PDE-MLaroundHPC: Learning Model Details (agents)

83. *MLaroundHPC: Learning Model Details (agents):* Use ANN's to discover the PDE form of biological transport equations from noisy data. [126]
84. *MLaroundHPC: Learning Model Details (agents):* Deep Learning to find sub-grid processes (such as cloud processes) for Climate prediction [127]

PDE-MLaroundHPC: Learning Model Details (coarse graining)

85. *MLaroundHPC: Learning Model Details (coarse graining):* Use of equation free modeling [128] for coarse graining combined with manifold learning (dimension reduction) [129]

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