

Computable Models (CompMods)
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I plan to report on DARPA's Computable Models program which aims to investigate and quantify the benefits of new and emerging mathematics and algorithms to enable direct generation of accurate and efficient multi-physics, multi-scale (time and space) simulation codes for complex physical systems relevant to DoD¹.

Accurate simulation codes for complex physical systems are generally not available from the commercial sector and have to be custom built. Building a custom code requires identifying the relevant physical phenomena and representing these phenomena through a set of equations. Current practice represents physical phenomena with Ordinary and Partial Differential Equations (ODEs, PDEs). In many complex systems, the ODEs and PDEs used to describe the relevant physical phenomena are generally not directly computable, meaning that neither a closed form solution exists, nor can a computer directly solve them over a given geometry. Converting these equations into computable discrete algebraic forms requires manual conversion by trained experts and can often introduce inaccuracies that are difficult to trace and quantify. Other approaches that model physics from the smallest scales (e.g., Direct Numerical Simulation) have shown to improve accuracy, but are limited by available compute power in simulating systems and platforms of relevant size. Because of this, the effort to build multi-physics simulation codes scales poorly with the number of interacting physics involved, making it very hard to represent all relevant physics needed to understand the behavior of complex physical systems.

New and existing ideas in mathematics and computer science such as discrete exterior calculus, machine learning, cellular automata, domain specific languages and software compilers have demonstrated a reduction in level of effort to develop physics codes such as Navier-Stokes and solid mechanics solvers by up to three orders of magnitude², >5x improvements in accuracy over SOA alternatives such as finite volume methods³ and >10x computational speedup in comparison to SOA methods in the simulation of turbulent fluids⁴ and electro-thermo-mechanical phenomena⁵. This presents an opportunity to rethink the process to create simulation codes that combine a larger number of physics (3 or greater) and multi-scale phenomena (10¹² scale range in space, 10¹⁵ scale range in time), improve accuracy (by over 5x) and reduce the time and level of effort to describe and generate a simulator (from years to weeks). These numbers serve as the target program metrics over SOA.

The Computable Models program aims to investigate and quantify the benefits of new and emerging mathematics and algorithms to enable direct generation of accurate and efficient multi-

¹ Michopoulos, J., Farhat, C., Fish, J., (2005). Modeling and Simulation of Multiphysics Systems. *J. Comput. Inf. Sci. Eng.*, 5(3), 198-213.² G.E. Karniadakis, DARPA AIRA Kick-Off, Feb 8, 2019, and: Raissi, M., Perdikaris, P., & Karniadakis, G. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378, 686–707. doi: 10.1016/j.jcp.2018.10.045

² G.E. Karniadakis, DARPA AIRA Kick-Off, Feb 8, 2019, and: Raissi, M., Perdikaris, P., & Karniadakis, G. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378, 686–707. doi: 10.1016/j.jcp.2018.10.045

³ Perot, J. B. (2011). Discrete Conservation Properties of Unstructured Mesh Schemes. *Annual Review of Fluid Mechanics*, 43(1), 299–318. doi: 10.1146/annurev-fluid-122109-160645

⁴ Barad, M., Kocheemoolayil J., Kiris C. (2017) *Lattice Boltzmann and Navier-Stokes Cartesian CFD Approaches for Airframe Noise Predictions*, AIAA-2017-4404 presentation.

⁵ Alotto, P., Freschi, F., Repetto, M., Rosso, C. (2013). The cell method for electrical engineering and multiphysics problems: an introduction. Heidelberg: Springer.

physics, multi-scale (time and space) simulation codes for complex physical systems relevant to DoD^{1,6}. The intent is to open up new approaches to accelerate the pace and accuracy at which modeling and simulations tools can be generated.

⁶ Keyes, D. C., McInnes, L. C., Woodward, C. C., Gropp, W. C., Myra, E. C., Pernice, M. C., ... Wohlmuth, B. (2013). Multiphysics simulations: challenges and opportunities. *Multiphysics Simulations: Challenges and Opportunities*, 27(1), 4–83. doi: 10.2172/1034263