SOFTWARE AND HARDWARE ACCELERATION STRATEGIES FOR CHEMICALLY REACTING, MULTI-PHASE SIMULATIONS OF AGENT DEFEAT SCENARIOS

Neeraj Sinha[1] and Andrea Zambon[2]

[1]CRAFT Tech, 6210 Keller's Church Road, Pipersville, PA 18947, USA
[2]CRAFT Tech, 6210 Keller's Church Road, Pipersville, PA 18947, USA

Key words: High fidelity simulations, chemical kinetics, software and hardware runtime acceleration

Abstract: High fidelity simulations of agent defeat is computationally intensive due to the long-time duration of interest (weapon detonation through vented plume stabilization), multi-scale phenomenology, turbulent mixing phenomena, the temperature dependency of thermal neutralization mechanisms, and the relatively stiff chemical kinetics models. Generalized multi-step chemical kinetics is necessary to represent the complexities of pyrolysis and oxidation for a wide range of H/C/N/O/P explosive and agent/simulant systems. Furthermore, modeling of multi-phase non-equilibrium mass / momentum / energy exchange between gases and dispersed particles/aerosol droplets is also required. As a result, computational resource requirements rapidly increase with scale and complexity to the point where "brute force" simulations on highly resolved spatial grids that may feature several 100 – 1000 million mesh elements become intractable since simulation time can easily approach several 10 – 100 seconds of physical time. As a result, high efficiency runtime software and hardware acceleration alternatives to the brute force strategy that retain physical accuracy and provide significant computational throughput have recently been investigated and assessed for applicability to this specialized application. A variety of such methodologies have been considered by the authors that address different aspects of the underlying simulation challenges, including:

1. **Skeletal and reduced models:** Utilizing sensitivity analysis, reaction pathway analysis, graph theory concepts and element flux maps to identify critical reaction pathways, dimensionality reduction of very large chemical kinetic mechanisms, dimensionality reduction is conducted to synthesize tractable chemical kinetic mechanisms.
2. **In-Situ Adaptive Tabulation (ISAT):** A tabulated approach is deployed to map chemical integration simulation solution to initial conditions for efficient storage and retrieval.
3. **Artificial Neural Networks (ANNS):** ANNS attempt to perform accurate functional fitting of the intrinsically high non-linearity, sensitivities and orders of magnitude variation of species mass fractions so that they may be subsequently deployed within CFD solvers in lieu of chemical kinetics evaluations.
4. **Tabulated Chemistry:** The Flamelet/Progress Variable (FPV) approach and its multi-time-scale (MTS) extension provides a significant breakthrough by radically reducing the number of scalars that must be transported, thereby providing dimensionality reduction and overcoming chemical stiffness.

5. **GPU and FPGA Acceleration:** The Graphical Processing Units (GPU) and Field Programmable Gate Arrays (FPGA) based runtime-acceleration hardware strategies leverage on chemistry data-parallelism to exploit their inherent advantage relative to the CPU.

The paper will provide illustrative applications of the above strategies to high fidelity simulations of agent defeat and highlight their efficiency gains relative to traditional brute-force methodology.