Predictive Simulations of Particle-Laden Turbulence in a Radiation Environment

Stanford University

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In 2013, the National Nuclear Security Administration (NNSA) selected Stanford University as one of the new centers of excellence in predictive science. Stanford was named as one of three Multidisciplinary Simulation Centers, under NNSA's Predictive Science Academic Alliance Program II (PSAAP II).

The project, "Predictive Simulations of Particle-Laden Turbulence in a Radiation Environment," focuses on the effect of radiation on particle motion in a turbulent airflow. This is a poorly understood physical process that can open new opportunities for efficiency gains in solar thermal receivers with applications in energy conversion and chemical splitting in hydrogen production plants. The objective in such systems is to achieve high temperatures with minimal losses to the environment. Conventional solar-receivers collect focused sunlight primarily via a solid surface, which then conductively heats a target fluid (see Figure 1). One main drawback is that achieving high mean temperature in the fluid requires local heating of the solid surface to even higher temperatures, which can result in significant radiation losses.

Particle-based receivers remedy this issue by allowing more uniform and volumetric absorption of radiation by the working fluid. Given most fluids are transparent to radiation, absorbing particles are needed to intercept high-energy solar rays and allow local transfer to the fluid mixture. However, the three-way coupled physics of particle transport, fluid dynamics, and radiation presents extraordinary challenges. For example, fluid motion in such systems naturally involves turbulence, and while turbulence helps global mixing of mass and heat, it induces preferential concentration of particles: local turbulent vortices can centrifuge out particles to zones of local shear, and lead to heating non-uniformities and reduction of the overall efficiency. Additionally, temperature inhomogeneity leads to local fluid expansion altering the turbulence structures. Insights into design and optimization of such systems require careful investigations of the physical interactions between particle, radiation transport, and fluid turbulence.

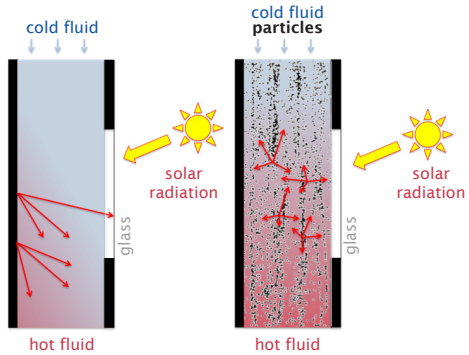

Figure 1. Heating of a mixture via a conventional receiver (left) and a particle-based receiver (right).

The Stanford PSAAP II Center is carrying out simulations at an unprecedented level of fidelity by accessing the largest supercomputers in the United States. A snapshot of one of the Center's high-resolution simulation is reported in Figure 2. The red spots in the temperature map represent local high-temperature air plumes generated by high radiation absorption, while the blue spots in the particle concentration plot show instantaneous preferential accumulation of solid particles driven by air turbulence. Such calculations will help develop and ultimately demonstrate predictive science on next-generation exascale systems—computers that can perform a trillion floating-point operations per second—expected to become available in 2020. The current trend in supercomputer systems is to increase the number of computing cores and, as a consequence, this leads to massive data movement across extensive networks. Moreover, diverse and specialized computing units (CPUs, GPUs, and other accelerators) and multiple memory banks with different performance will coexist creating a truly complex hardware and network system. Achieving high performance requires new programming models that enable computational scientists to develop algorithms and software tools without intimate knowledge of the underlying architecture details. A key feature of the Center is the strong partnership between computational and computer scientists. Domain Specific Languages such as

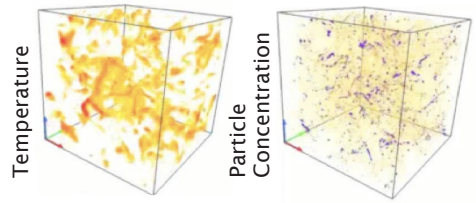

Figure 2. Instantaneous snapshot from direct numerical simulation of radiation-induced turbulence in a particle-laden fluid.

Stanford's developed Liszt are the key ingredient to enable computer programs to identify and recover from faults while providing flexibility in data management and efficiency in mapping simulation algorithms on the most appropriate computing units.

The project will also concentrate on uncertainty analysis, allowing researchers to quantify errors and uncertainties in the simulations and, therefore, to determine how much confidence can be placed in the results. A dedicated experimental campaign will be undertaken alongside the computational work to help understand and identify these uncertainties and to provide overall validation data to assess the predictive ability of the physical models and soft-ware tools developed within the project.

Broad interdisciplinary knowledge spanning energy systems, fluid dynamics, radiation physics, and multiphase flow systems is required to tackle Stanford's PSAAP problem. The project provides opportunities for collaborations with the NNSA national laboratories and, in addition, the research activities also impact the graduate curriculum at Stanford with the introduction of new courses on multiphase flow and radiation modeling. Further impact on the simulation technology across computer science, numerical analysis, and statistical sciences is also anticipated.

The project continues a 15-year history of strong collaboration between NNSA national laboratories and Stanford University, including the Advanced Simulation and Computing and PSAAP programs.