Efficient Use of HPC Resources for Turbulent Mixing Simulations

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I use Blue Waters to

- motivate and train University of Arkansas undergraduate students in the use of large-scale computation and data analytics.
- optimize and scale Front Tracking application code to large-scale turbulent mixing simulations.

Rayleigh–Taylor hydrodynamic interface Instability

an idealized subproblem of important scientific and engineering problems

- crucial in all forms of fusion whether the confinement be magnetic, inertial or gravitational : inertial confinement fusion, supernovae explosions
- predict growth rate, α, that describes the outer edge of the mixing zone

$$h_b = \alpha A g t^2$$

h_b, penetration distance of the light fluid into the heavy fluid

A, Atwood ratio $= (\rho_2 - \rho_1)/(\rho_2 + \rho_1)$

g, acceleration

- Validation and Verification (V&V) : Quantifying errors and uncertainties in multi-physics models and data are crucial to achieve good V&V results for the numerical simulations of realistic applications.
  Glimm-Cheng-Sharp-Kaman 2019
- Uncertainty Quantification Analysis : dependence of α_b on the experimental parameters, such as width of initial mass diffusion layer, long wavelength initial perturbations, fluid viscosities. *Kaman-2018*
- Numerical models for turbulent flows :
  - Reynolds Averaged Navier Stokes (RANS) :
    - resolve length scales sufficient to specify the problem geometry
    - time-averaged equations solving for the mean values of all quantities
    - the least demanding in terms of resources
  - Large Eddy Simulation (LES) :
    - resolve these scales, and also resolve some of the generic turbulent flow
  - Direct Numerical Simulation (DNS) :
    - resolve all relevant length scales
    - full NSE is solved without any model for turbulence
    - the most demanding in terms of resources, very accurate, but limited to moderate Reynolds numbers and simplified geometries

Sensitivity to both the modeling issues and the algorithmic issues

The essential features of our algorithmic strategy (LES/SGS/FT) are twofold :

- front tracking (FT) to control numerical mass diffusion (achieve resolution of sharp interfaces or steep gradients)
- LES with dynamic subgrid models (SGS) to account for the effects of the unresolved scales on the resolved ones.
  - Filtered continuity, momentum, energy and concentration equations for compressible flow
  - Because the equations are nonlinear, the averaging produces an error

$$\text{Reynolds Stress} = \overline{vv} - \overline{v}\,\overline{v}\ .$$

  - The difference is approximated by a term proportional to a gradient ; the coefficient of proportionality in SGS models are determined from the simulation itself, the models are parameter free.

These features are included in the multipurpose simulation code **FronTier**.

Model : Multispecies Navier-Stokes equations

The filtered continuity, momentum, energy, and concentration equations :

$$
\begin{aligned}
&\frac{\partial\overline{\rho}}{\partial t}+\frac{\partial\overline{\rho}\widetilde{v_i}}{\partial x_i}=0\ ,\\
&\frac{\partial\overline{\rho}\widetilde{v_j}}{\partial t}+\frac{\partial(\overline{\rho}\widetilde{v_i}\widetilde{v_j}+\overline{p}\delta_{ij})}{\partial x_i}=\frac{\partial\overline{d_{ij}}}{\partial x_i}-\frac{\partial\tau_{ij}}{\partial x_i}\ ,\\
&\frac{\partial\overline{E}}{\partial t}+\frac{\partial(\overline{E}+\overline{p})\widetilde{v_i}}{\partial x_i}\ =\frac{\partial\overline{d_{ij}}\widetilde{v_j}}{\partial x_i}+\frac{\partial}{\partial x_i}\left(\overline{\kappa}\frac{\partial\widetilde{T}}{\partial x_i}\right)+\frac{\partial}{\partial x_i}\left((\widetilde{H_h}-\widetilde{H_l})\overline{\rho}\widetilde{D}\frac{\partial\widetilde{\Psi}}{\partial x_i}\right)\\
&+\left(\frac{1}{2}\frac{\partial\tau_{kk}\widetilde{v_i}}{\partial x_i}-\frac{\partial q_i^{(H)}}{\partial x_i}-\frac{\partial q_i^{(T)}}{\partial x_i}-\frac{\partial q_i^{(V)}}{\partial x_i}\right)\ ,\\
&\frac{\partial\overline{\rho}\widetilde{\Psi}}{\partial t}+\frac{\partial\overline{\rho}\widetilde{\Psi}\widetilde{v_i}}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\overline{\rho}\widetilde{D}\frac{\partial\widetilde{\Psi}}{\partial x_i}\right)-\frac{\partial q_i^{(\Psi)}}{\partial x_i}\ .
\end{aligned}
$$

The dependent filtered variables $\overline{\rho},\widetilde{\Psi},\widetilde{v_i},\overline{p}$, and $\overline{E}$ the total mass, the species mass fraction, the velocity, the pressure and the total specific energy, with

$$\overline{E}=\overline{\rho}\widetilde{e}+\overline{\rho}\widetilde{v_k}^2/2+\tau_{kk}/2$$

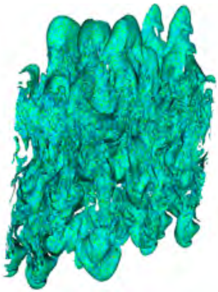
$\widetilde{H_h}$ and $\widetilde{H_l}$ are the partial specific enthalpy of each species defined by

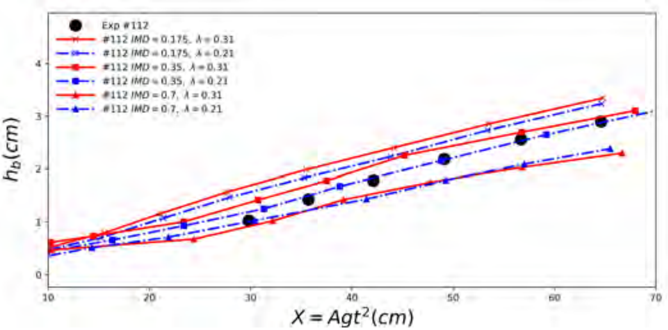
$$\widetilde{H_h}=\widetilde{e_h}+\frac{\overline{p}}{\overline{\rho}},\qquad \widetilde{H_l}=\widetilde{e_l}+\frac{\overline{p}}{\overline{\rho}}\ ,$$

where $\widetilde{e_h}$ and $\widetilde{e_l}$ are the specific internal energy of each species.

V&V of turbulence simulations - I

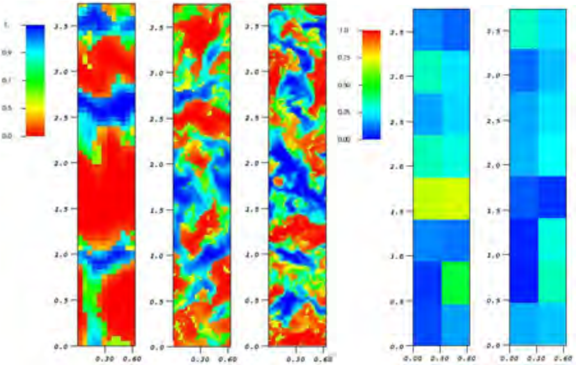
Ref.	Exp.	α_{exp}	α_{sim}
Smeeton Youngs 87	#112	0.052	0.055
Smeeton Youngs 87	#105	0.072	0.076 ± 0.004
Smeeton Youngs 87, Read84	10 exp.	0.055-0.077	0.066
RamAnd04	air-He	0.065-0.07	0.069
Mueschke 08	Hot-cold	0.070 ± 0.011	0.075
Mueschke 08	Salt-fresh	0.085 ± 0.005	0.084





V&V of turbulence simulations - II

- Left : Heavy fluid concentration at the midplane
- Right : Spatial array L_1 norms of CDF mesh differences



Application code **FronTier**

- mature, production-quality multiphysics simulation package and under continuous development
- pure-MPI : to pass states and interface data from one processor to another.
- scales to the entire system on Argonne's IBM Blue Gene/P supercomputer (Intrepid) - 62% efficiency on 163,840 cores. INCITE 2011-2012.
- computational intense large-scale simulations on Cray XC50 system installed at the Swiss National Supercomputing Centre (CSCS), 5th place in November 2018.

Education Allocation :

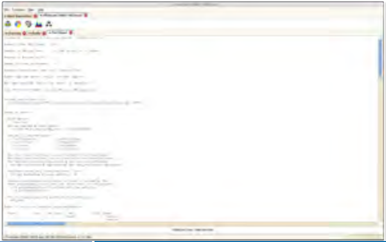
- Programming Environments : Cray/ GNU/ Intel/ PGI compilers
- Profilers : identify the performance bottlenecks (CPMAT + TAU)
- Tune the front tracking application code FronTier on BlueWaters
- Develop Hybrid (MPI+OpenMP) parallelization strategies and perform scaling studies

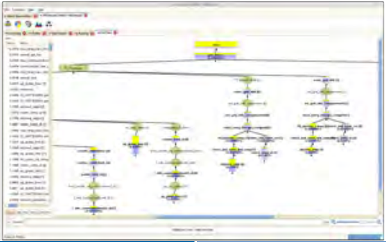
Profilers

1. Cray Performance Measurement and Analysis Tools (CPMAT)
2. The TAU Parallel Performance System
   `https://www.cs.uoregon.edu/research/tau`

- Instrument the source code
- Execute the generated executable
- View the parallel profile results

Cray Performance Measurement and Analysis Tools (CPMAT)

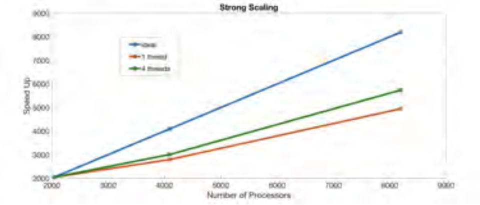


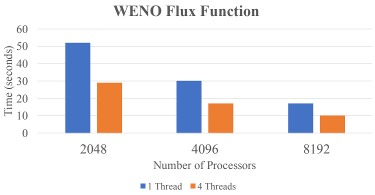


The TAU Parallel Performance System

Hybrid MPI and OpenMP

- combine communication with computation with MPI built-in collective computation operations
- implement the parallel formulation by the OpenMP library routines for fifth order Weighted Essentially Non-Oscillatory (WENO) scheme
- investigate OpenMP scheduling





Shu. High order weighted essentially nonoscillatory schemes for convection dominated problems. SIAM Review, 2009.

Blue Waters

- is used to run many of the computationally intense simulations
- supported me in guiding and teaching two University of Arkansas undergraduate students
  - participate in two-week intensive Petascale Institute at the NCSA on the University of Illinois Urbana-Champaign campus, May 21 - June 1, 2018.
  - receive travel awards to SC18 International Conference for High Performance Computing, Networking, Storage, and Analysis in Dallas, Texas, November 11-16, 2018.

Presentations

- J. McGarigal (Poster), *NCSA 2019 Blue Waters Symposium*, Sunriver, OR, June 3–6, 2019.
- J. McGarigal (Poster), *2019 Arkansas Academy of Science*, Hendrix College, AR, March 29-30, 2019. (1st Place Undergraduate Poster, Computer Science)
- A.Edwards (Talk), *2019 Arkansas Academy of Science*, Hendrix College, AR, March 29-30, 2019.
- A. Edwards (Poster), *American Physics Society Conference for Undergraduate Women in Physics*, Texas A&M University at Corpus Christi, TX, January 18–20, 2019.

A. Edwards, J. McGarigal, student paper to the Journal of Computational Science Education, in preparation.

U of A Undergraduate Students, 2018-2019 Blue Waters Interns
Alaina Edwards : Summer 2019 Oak Ridge National Lab Intern
John McGarigal : Summer 2019 Texas HP Inc. Intern

Collaborators :

J. Glimm, Stony Brook University, NY.

B.Cheng and D. H. Sharp, Los Alamos National Laboratory, Los Alamos NM.

References :

- H. Zhang, T. Kaman, D.She, B. Cheng, J. Glimm and D. H. Sharp, V&V for turbulent mixing in the intermediate asymptotic regime, Pure and Applied Mathematics Quarterly, Vol. 14, No. 1, pp. 193-222, 2018.
- T. Kaman, Model calibration for Turbulent Mixing Simulations, Proceedings of 16th International Workshop on the Physics of Compressible Turbulent Mixing, pp.129-134, Marseille, France, July 15-20, 2018.
- J. Glimm, B. Cheng, D. H. Sharp and T. Kaman, A crisis for the verification and validation of turbulence simulations, Physica D : Nonlinear Phenomena, submitted May 2019.

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