

Summary:

The overall scalability of an adaptive algorithm is highly dependent on the scalability of its intermediate states. Intermediate states may be unscalable if the domain decomposition is not good.

A scalable state is characterized by:

- $T_{comp} \gg T_{comm}$ and
- $T_{comm} \sim t_{tr}$, where t_{tr} is the data transfer time.
- The fundamental reason here is that both T_{comm} and t_{tr} decrease with subdomain size, i.e. as p increases, while the global problem size remains constant.
- Note: $T_{comp} \sim (p^{-1})$ and $T_{comm} \sim (p^{-1/2})$, so as p increases $T_{comm}/T_{comp} > 1$.

An unscalable state is characterized by:

- $T_{comp} \sim T_{comm}$ (sufficient condition)
- $T_{comm} \sim t_{sync}(\sigma_{comp})$ when the shortcomings of the domain decomposition affect scalability.
 - § Note: This is not a sufficient condition.
 - § A better domain decomposition will solve the problem.

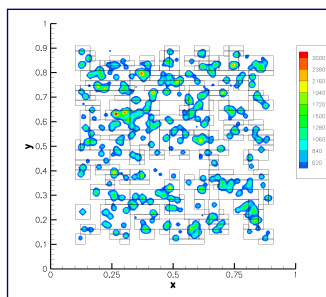
Acknowledgements:

Our research is funded by the U.S. Department of Energy:

- Office of Basic Energy Sciences: SciDAC Computational Chemistry Program
- Office of Advanced Scientific Computing Research: MICS

Test case:

2D Reaction-Diffusion with detailed H_2 -Air chemistry using SAMR with three levels of refinement (RF=2). The initial condition is a random kernel temperature field with stoichiometric composition.



We integrate in time solving implicitly for chemistry and explicitly for diffusion. We perform timings at two different timesteps corresponding to two very different states of the simulation.

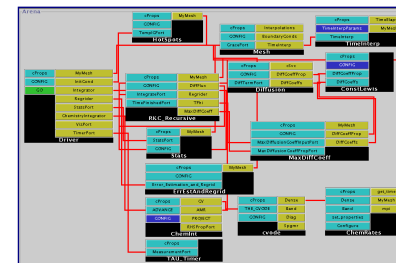
URLS:

- <http://cfrfs.ca.sandia.gov>
- <http://www.cs.uoregon.edu/research/paracomp/tau>
- <http://www.cca-forum.org>
- <http://www.scidac.org>

Software:

Our software toolkit is CCA (Common Component Architecture) compliant, build with individual modules which perform distinct functionalities.

- Mesh Generator: componentized GrACE
- Explicit subsystem for Diffusion: Runge-Kutta Chebyshev integrator, Constant Lewis Number diffusion coefficients.
- Implicit subsystem for chemistry: componentized CVODE, ChemRates.
- Profiling: componentized TAU.



Our runs were performed on the platinum cluster at NCSA, UIUC.