Project Report - Cordero, Maric, Seravalli

Features

- Chemical transport
  - Diffusion
  - Advection
  - Arbitrary position of chemical sources
- Chemical reactions
  - aA + bB -> cC + dD (direct reaction)
  - aA + bB <-> cC + dD (reversible)
  - Temperature dependency
  - Arbitrary number of chemicals
  - Catalysts
- Shared memory parallelization

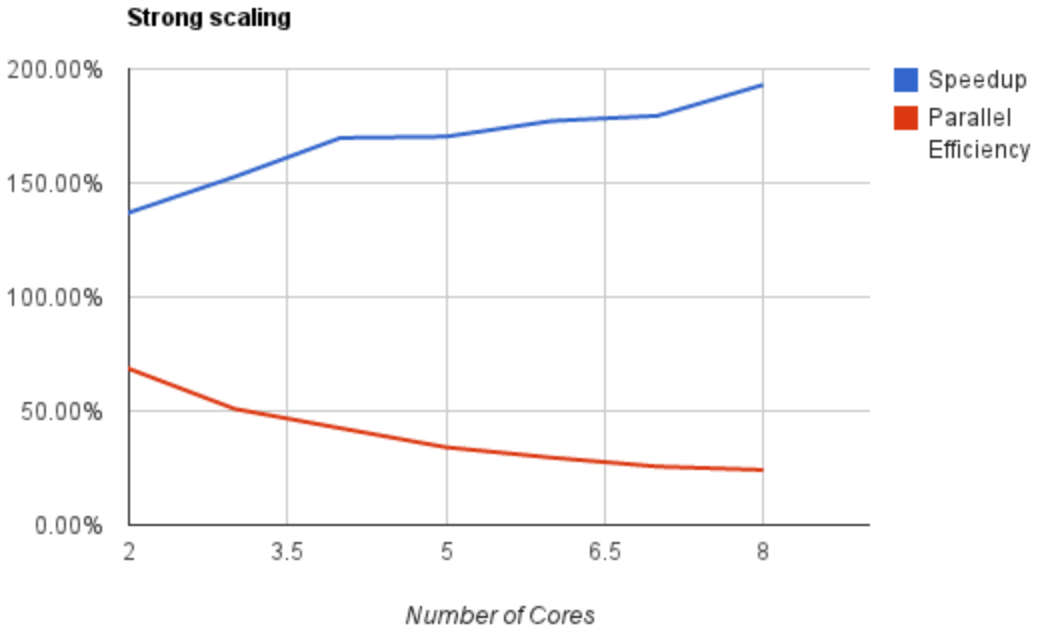
Test cases

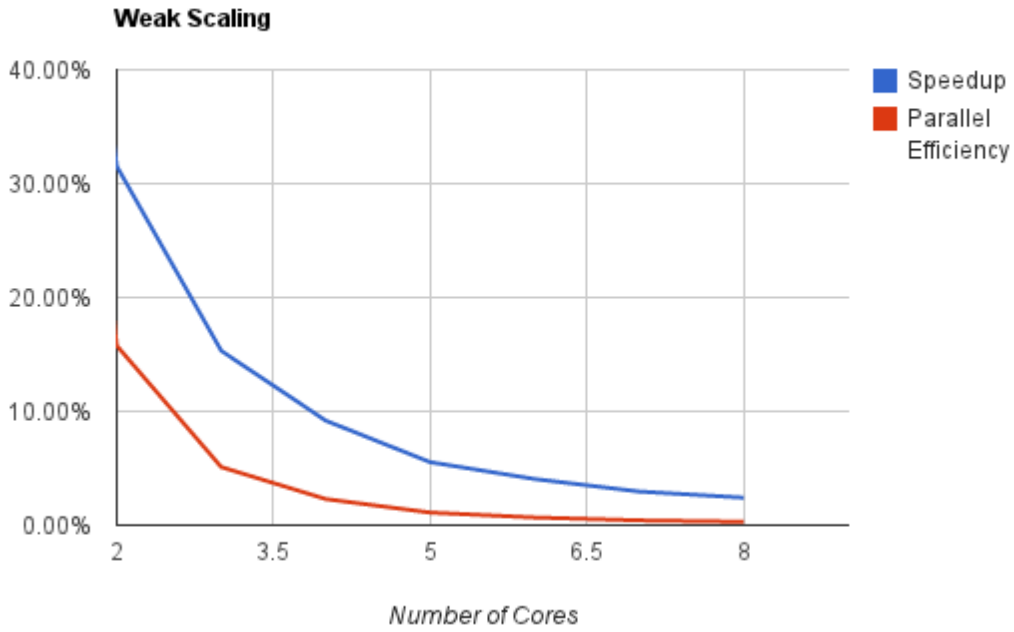
- Scenario 1: in the proposed scenarios two substances are released, a first one from the upper left corner and a second one from the lower left corner, the two substances will react to create a third one; a set of obstacle is placed in the middle of the scenarios to simulate a solid porous catalyst
  - Catalytic structure without catalyst: only the structure is added, without influence over the chemical reaction
    - $ export OMP_NUM_THREADS=8; ./sim noCatalystIrreversible
    - Expected outcome: increase of amount of third substance and decrease of reactants
  - Catalytic structure with catalyst: fluid cells surrounding the catalyst will be affected by an increase in the reaction
    - $ export OMP_NUM_THREADS=8; ./sim catalystIrreversible
    - Expected outcome: increase of amount of third substance and decrease of reactants, the amount of the third substance is higher than in the previous case
  - Catalytic structure with catalyst and reversible reaction: fluid cells surrounding the catalyst will be affected by an increase in the reaction, the reaction is reversible (aA + bB <-> cC)
    - $ export OMP_NUM_THREADS=8; ./sim catalystReversible
    - Expected outcome: after the higher production of the third substance within the catalytic area, the amount will decrease in the right part of the scenario thanks to the reversible reaction in order to reach an equilibrium
- Scenario 2: in the proposed example a baffle structure is included, there are some barriers that constrain the fluid to a specific path; two substances are input in the scenario and a third one will be created from the former two
  - Lower temperature: the temperature of the scenario is set to 350 Kelvin
    - $ export OMP_NUM_THREADS=8; ./sim baffleLowerT
    - Expected outcome: the two substances will progress through the structure creating the product, at the current temperature the direct reaction is favoured (aA + bB -> cC)
  - Higher temperature: the temperature of the scenario is set to 370 Kelvin
    - $ export OMP_NUM_THREADS=8; ./sim baffleHigherT
    - Expected outcome: the two substances will progress through the structure creating the product, at the current temperature the inverse reaction is favoured (aA + bB <- cC)

Scalability results

For testing the scalability all the calculations of F, G, RHS, C, T and Q were merged into a single function to reduce the forks and joins. The changes are not included in the provided code for readability reasons. The best results had been obtained by adopting a static scheduling with a predefined chunk size, which was approximately the number of cells per core.

The results of strong and weak scaling can be seen in the charts below





The result from all experiments can be seen in the attached xml file.

Note: all the simulations will write the vtk files in the vtk directory. Only the fluids immediately close to the catalytic obstacles are influenced.