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MULTI-LEVEL TECHNIQUES FOR THE SOLUTION OF THE KINETIC EQUATIONS IN CONDENSING FLOWS

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CONTENTS

- Introduction
- Theory
- Test case: Nucleation pulse
- Conclusions & recommendations

WHAT IS CONDENSATION
INTRODUCTION

Condensation: transition of fluid from gaseous to liquid phase

WHAT IS CONDENSATION

INTRODUCTION

- Condensation consists of
  - **Nucleation**, individual vapor molecules form clusters
  - Growth, *stable* clusters grow further

- Characteristic parameter condensation process: supersaturation S

$$S = \frac{p_v}{p^S(T)}, \quad S = 1$$ is called saturated

- Minimum size n for *stable* clusters is critical cluster size n_{cr}
- For $S = 1$, $n_{cr} = \infty$ → all clusters are unstable

TYPES OF NUCLEATION
INTRODUCTION

Heterogeneous nucleation

Homogeneous nucleation

SINGLE- VS. MULTI-COMPONENT CONDENSATION

INTRODUCTION

- Single-component condensation
  - One condensable component present
  - Droplets consist of a single substance
  - Relatively simple

- Multi-component condensation
  - Multiple condensable components present
  - Variable droplet composition
  - Considerably more complex

- A first step is to investigate single-component condensation

RESEARCH QUESTION
INTRODUCTION

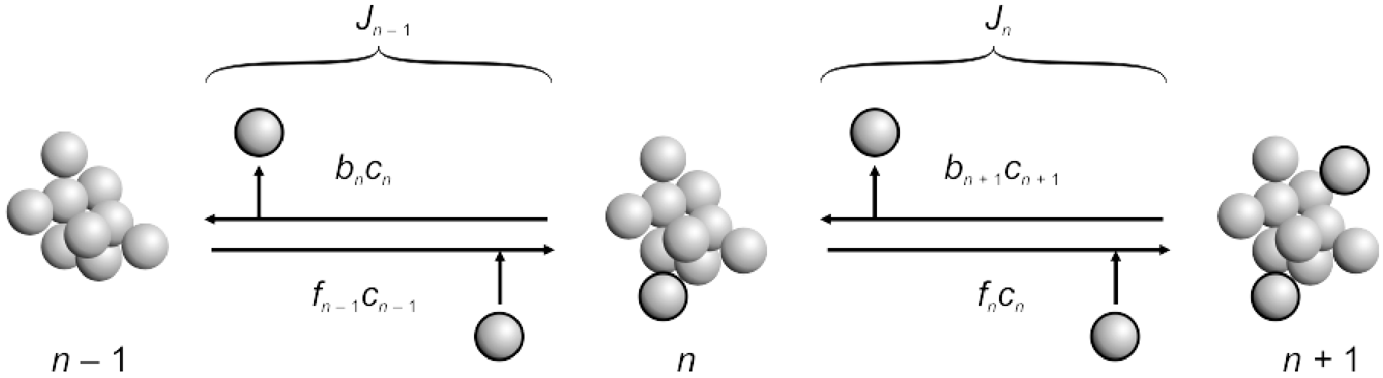
- Accurate numerical solution of condensation process: extremely long computer run times
- Multi-level methods can lead to very efficient algorithms for numerical solution

Can multi-level methods help in the numerical solution of condensation?

THEORY

- Introduction
- Theory
  - The Kinetic Equation
  - Multi-level methods
  - Application
    - Coarsening
    - Global constraint
- Test case: Nucleation pulse
- Conclusions & recommendations

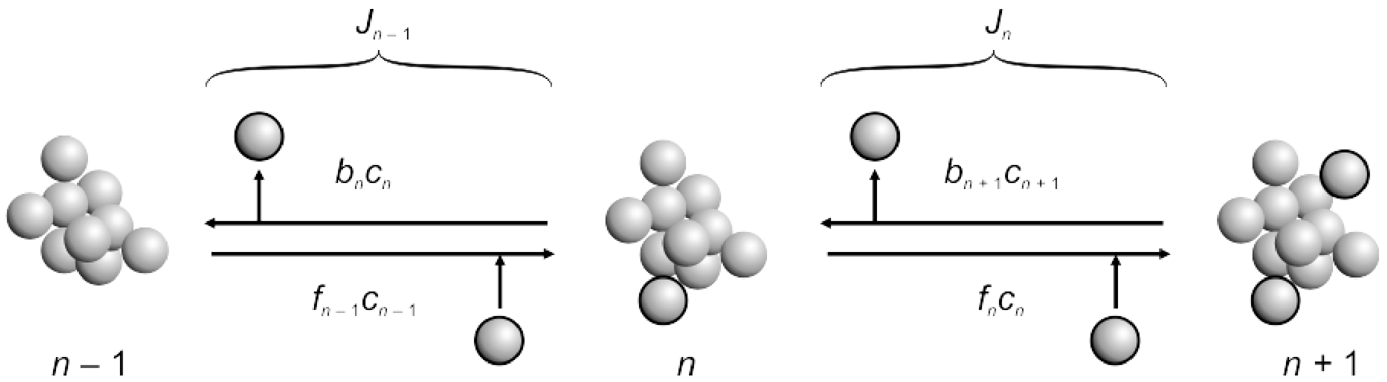
THE KINETIC EQUATION (KE)
THEORY



- Droplets grow or decay through interaction with monomers
- KE describes time rate change of volumetric number density c_n [#/m³]
- Changes described by forward (condensation) rates f_n and backward (evaporation) rates b_n

$$\frac{\partial c_n}{\partial t} + \frac{\partial u_j c_n}{\partial x_j} = J_{n-1} - J_n, \quad n = 2,3,\ldots,\infty \quad \text{with } J_n = f_n c_n - b_{n+1} c_{n+1}$$

THE KINETIC EQUATION (KE)
THEORY



- Result: $$\frac{\partial c_n}{\partial t} + \frac{\partial u_j c_n}{\partial x_j} = f_{n-1} c_{n-1} - (b_n + f_n) c_n + b_{n+1} c_{n+1}, \quad n = 2,3,\ldots,\infty$$

- Forward rates and backward rates are function of:
  - Monomer density c_1
  - Supersaturation S
  - Droplet size n
  - Temperature T

THE KINETIC EQUATION (KE)
THEORY

- Two options for monomer number density c_1
  - Fixed c_1
  - c_1 depletes with formation of droplets

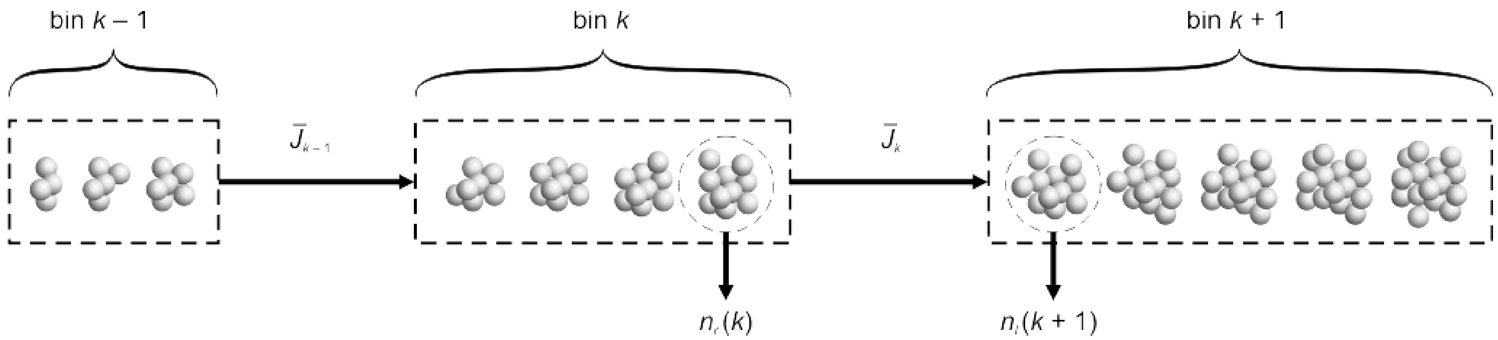
- First option results in Dirichlet boundary condition
- Second option adds extra equation, depending on *all* variables c_n:

$$\gamma \equiv \sum_{n=1}^{N} n c_n, \quad \gamma$$ = total monomer number = constant

THE KINETIC EQUATION (KE)

THEORY

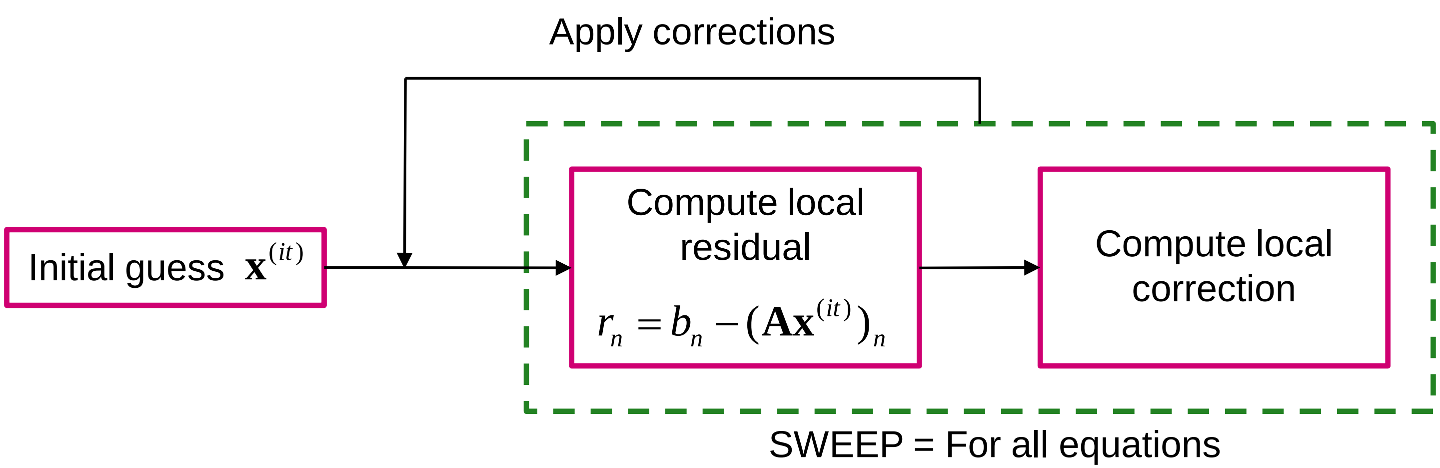
- Typically, practical cases include droplets up to a 100 million monomers
- Number of equations can be reduced by grouping ranges of droplet sizes



- Computation of average bin densities $\bar{c}_k$

MULTI-LEVEL METHODS
THEORY

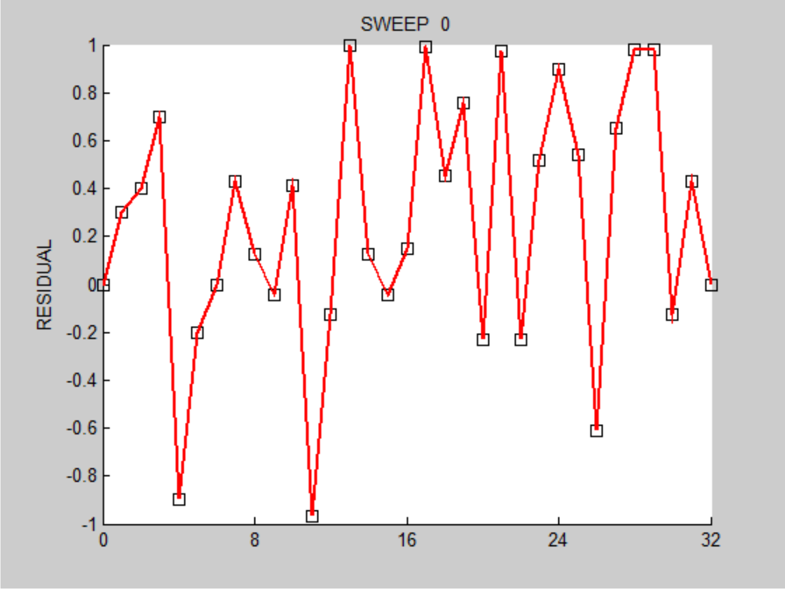
- System of N equations $\mathbf{Ax} = \mathbf{b}$
- Multi-level method is iterative process, based on relaxation:



- Computation time for relaxation: $O(N)$ iterations or $O(N^2)$ operations
- Multilevel-methods achieve $O(1)$ iterations or $O(N)$ operations

MULTI-LEVEL METHODS
THEORY

- Residual reduction for 1D Laplace's equation: $\frac{d^2\mathbf{c}}{dx^2} = \mathbf{0}$ (3-point operator)

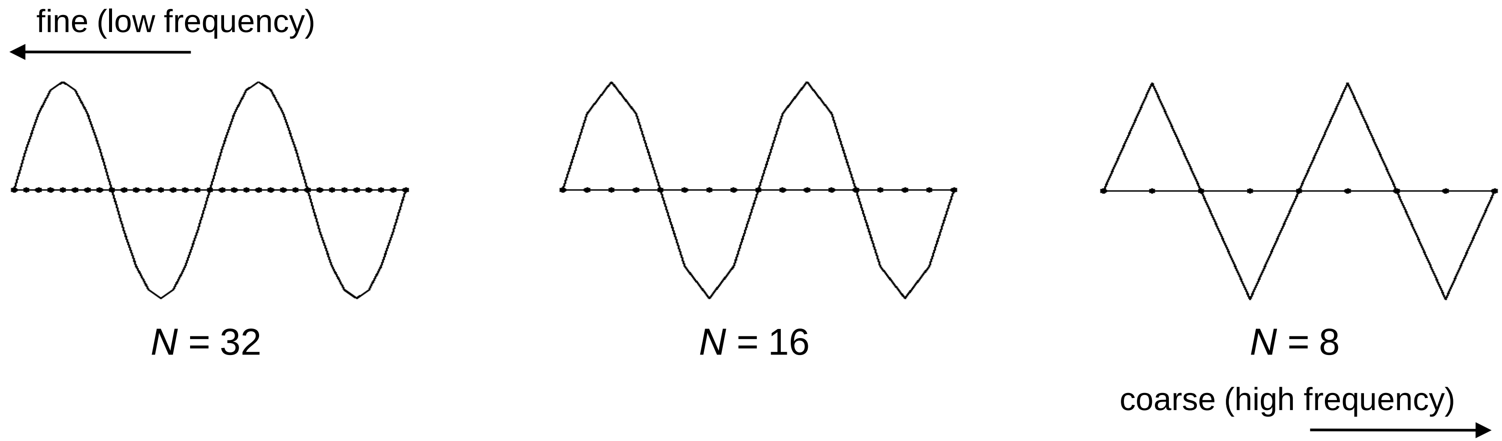


Gauss-Seidel relaxation

- <u>Low frequency components hardly seen by 3-point operator</u>

MULTI-LEVEL METHODS
THEORY

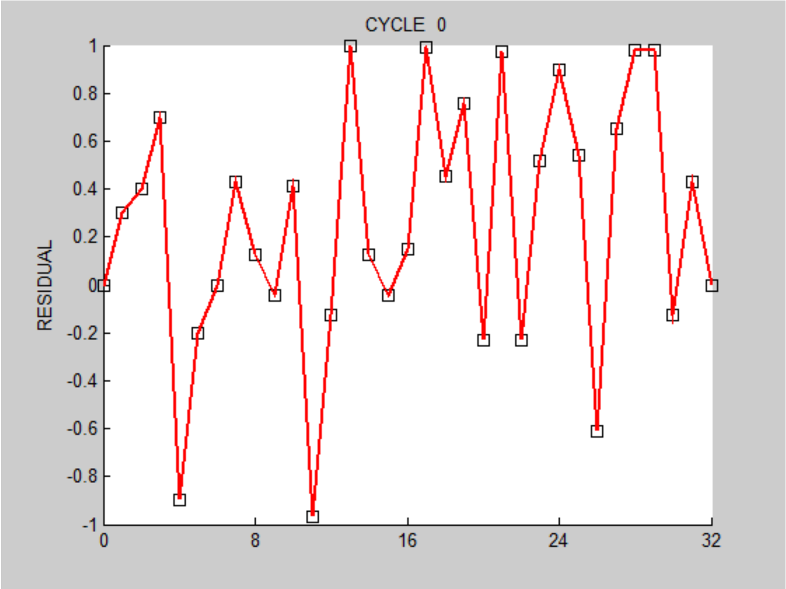
- Remedy: Represent low frequency components on coarser grids



- Multi-level methods employ relaxation on different grids
- All scales in error are treated effectively appropriate grids

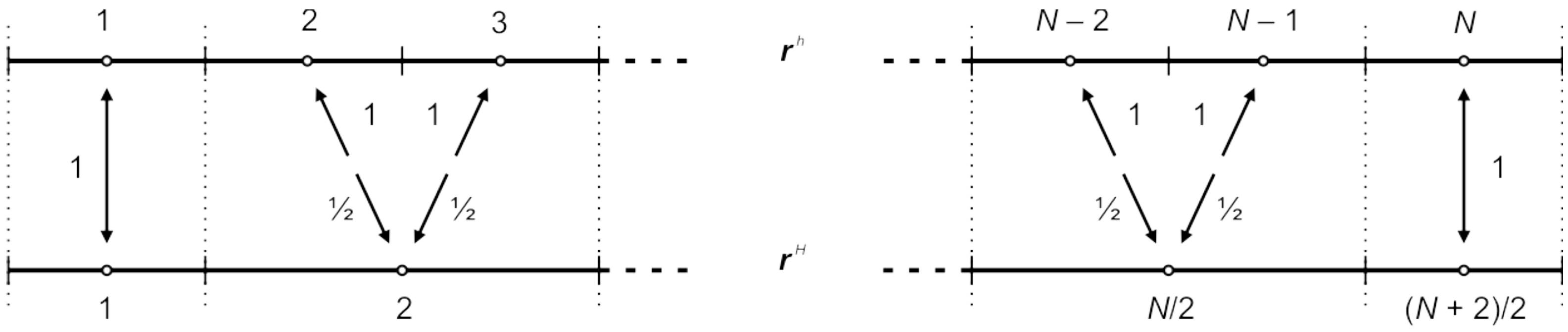
MULTI-LEVEL METHODS
THEORY

- Residual reduction for 1D Laplace's equation: $\frac{d^2\mathbf{c}}{dx^2} = \mathbf{0}$



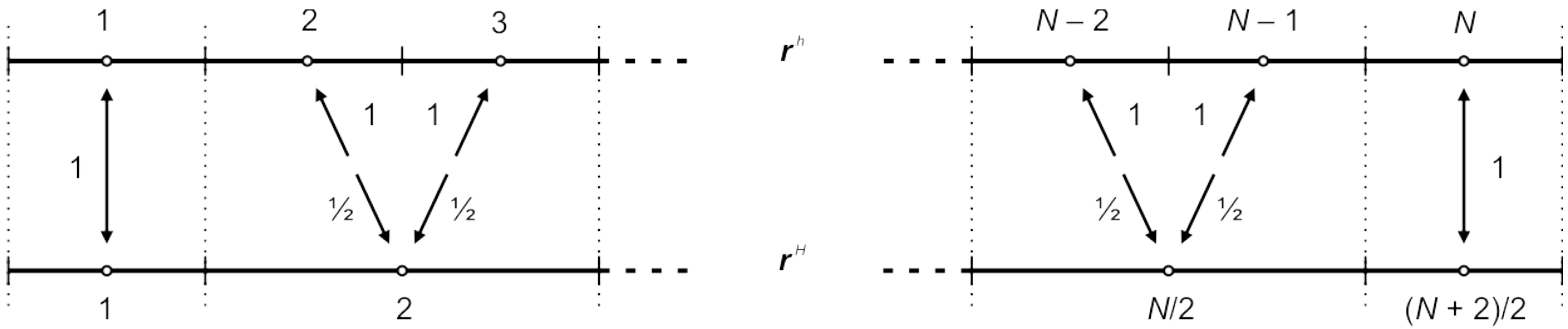
Multi-level cycles

APPLICATION: COARSENING
THEORY



- Cell-centered coarsening
- Variables located at cell centers
- Coarse grid cells edges coincide with target cell edges

APPLICATION: COARSENING
THEORY



- Cell-centered coarsening matches definition of KE
  - Consistent 3-point operator for all grids
  - Properties of KE preserved on different grids
  - Relaxation method can be applied on all grids

APPLICATION: GLOBAL CONSTRAINT
THEORY

- Formation of droplets depletes the amount of monomers according to:

$$\gamma \equiv \sum_{n=1}^{N} n c_n \rightarrow \boxed{c_1 = \gamma - \sum_{n=2}^{N} n c_n}$$

- Change in c_1 yields global changes:
  - Supersaturation S
  - Forward and backward rates f_n and b_n
- Depletion equation is a global constraint

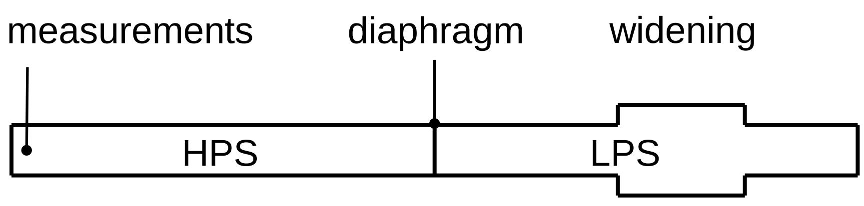
- Global constraint is applied after each *target* level relaxation sweep

TEST CASE: NUCLEATION PULSE

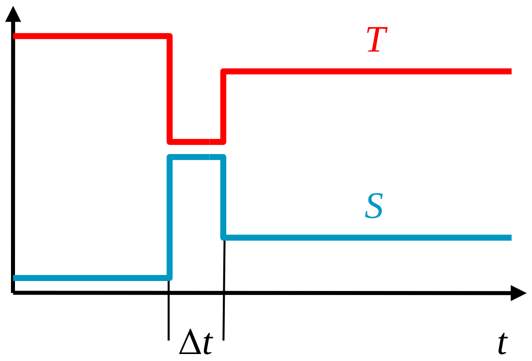
- Introduction
- Theory
- Test case: Nucleation pulse
  - Description
  - Results
    - Without depletion
    - With depletion
- Conclusions & recommendations

DESCRIPTION

TEST CASE: NUCLEATION PULSE



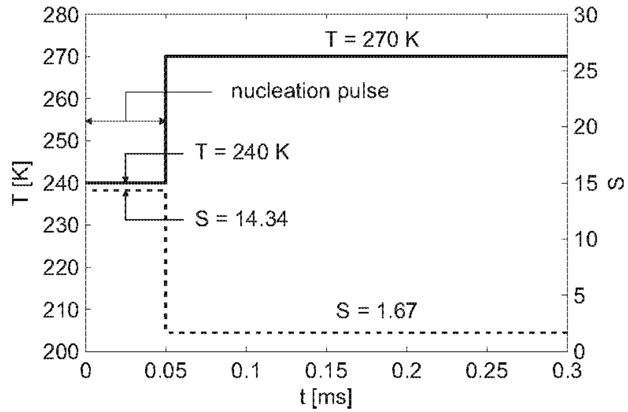
Expansion-wave tube



- Expansion-wave tube creates nucleation pulse for short period
- Supersaturation levels are changed by adjusting widening

DESCRIPTION

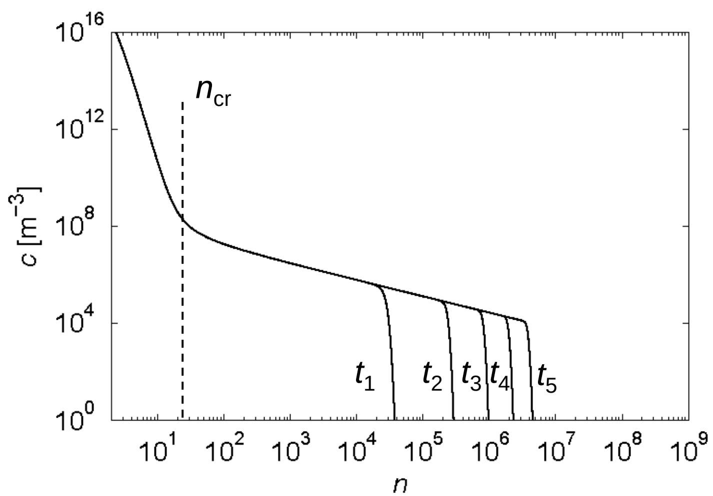
TEST CASE: NUCLEATION PULSE



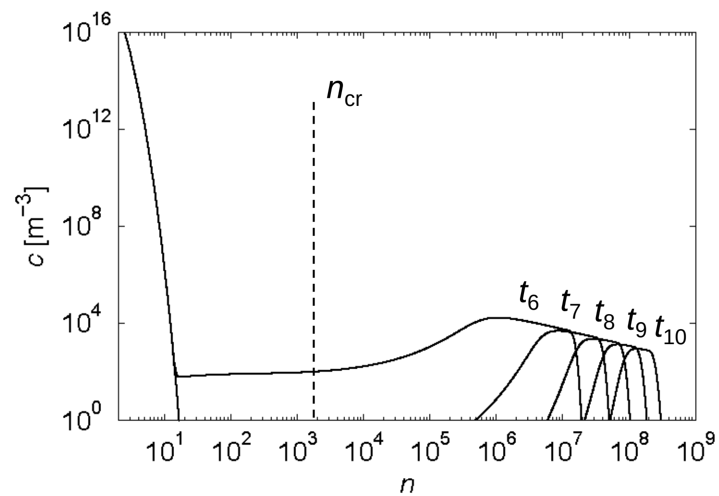
- No advection: second-order time-marching algorithm
- Relaxation/multi-level cycle is applied each time step
- Solution previous time step is initial guess for next time step

- One-way coupled: Effects of latent heat release are neglected

RESULTS: WITHOUT DEPLETION
TEST CASE: NUCLEATION PULSE



Expansion, S = 14.34
t = 10, 20, 30, 40, 50 μs



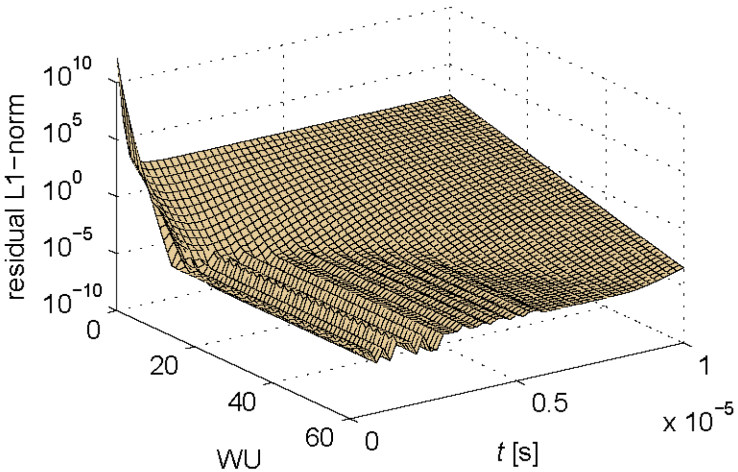
Compression, S = 1.67
t = 100, 150, 200, 250, 300 μs

- Expansion: Supersaturated conditions
  - Many stable clusters
  - The solution only changes at the nucleation front
- Compression: Near saturated conditions, few stable clusters can grow

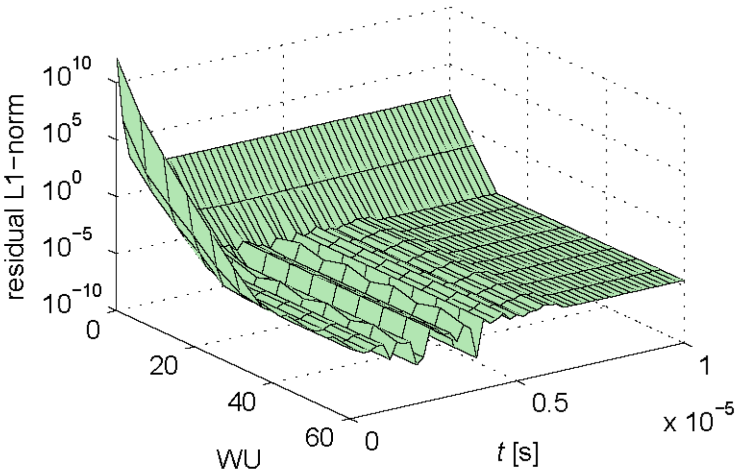
RESULTS: WITHOUT DEPLETION

TEST CASE: NUCLEATION PULSE

- Full KE: Residual reduction during expansion stage



Relaxation

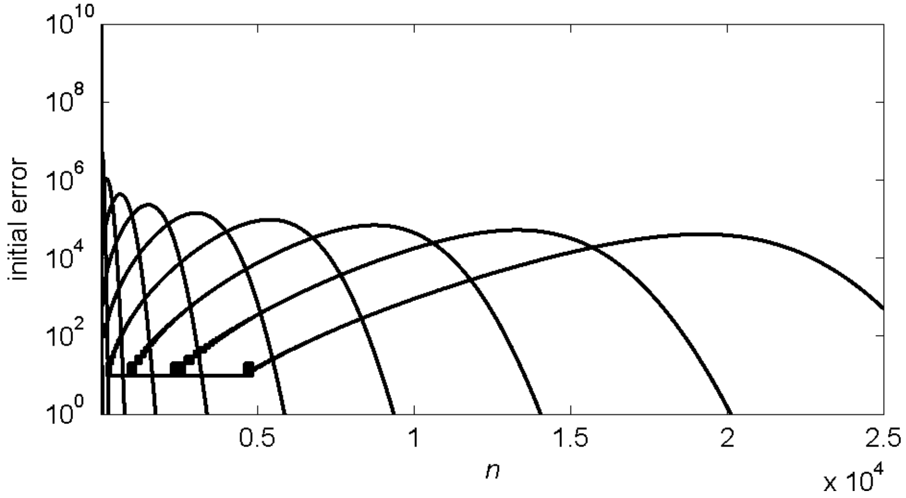


Multi-level cycles

- <u>Multi-level cycling is more effective over time</u>

RESULTS: WITHOUT DEPLETION
TEST CASE: NUCLEATION PULSE

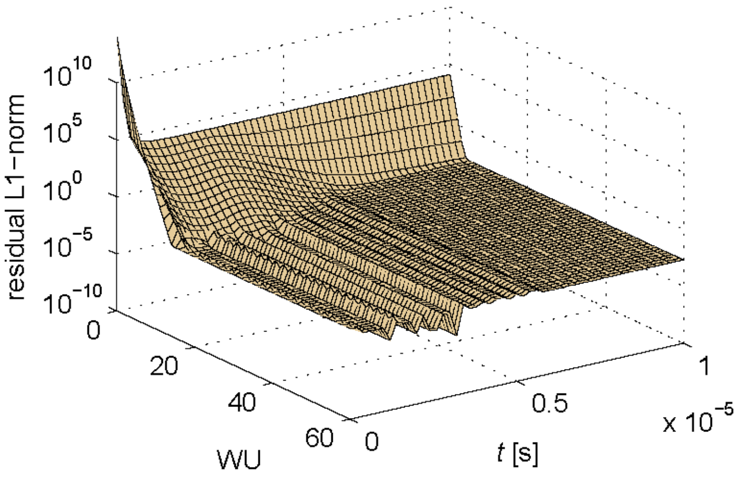
- Full KE: initial error at different time steps



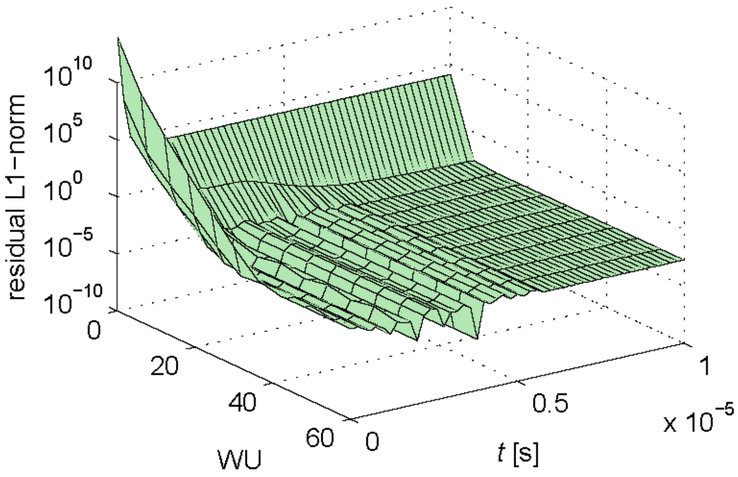
- Initial errors are present at nucleation front
- The front advances faster with time
- This results in lower frequency of error

RESULTS: WITHOUT DEPLETION
TEST CASE: NUCLEATION PULSE

- Binned KE: Residual reduction



Relaxation

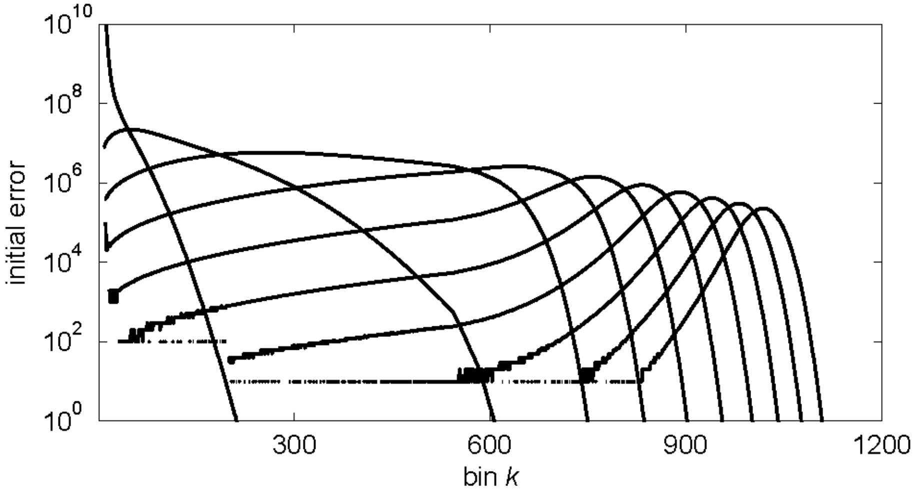


Multi-level cycles

- <u>Multi-level cycling performs similar</u>

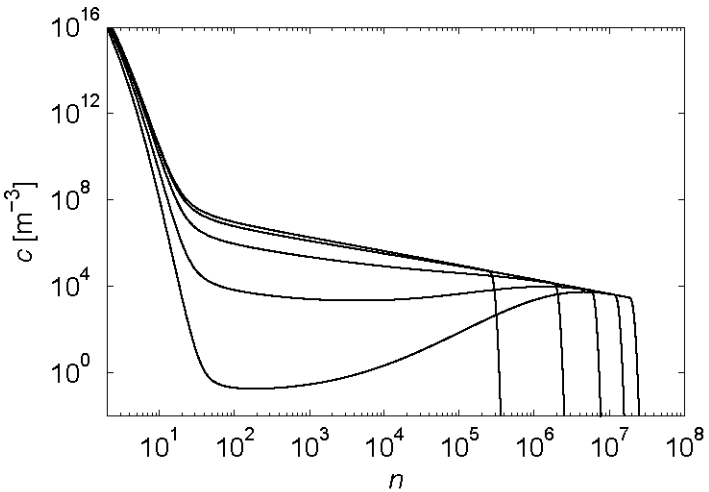
RESULTS: WITHOUT DEPLETION
TEST CASE: NUCLEATION PULSE

- Binned KE: initial error at different time steps

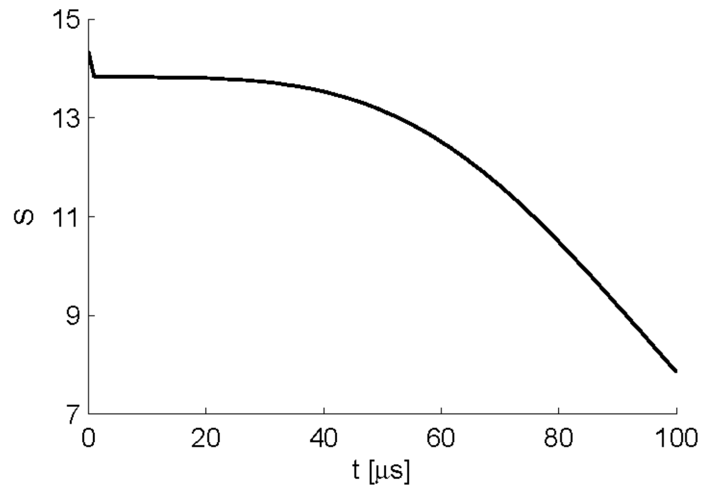


- Choice of grid matches advancement of nucleation front
- Initial errors remain of high frequency

RESULTS: WITH DEPLETION
TEST CASE: NUCLEATION PULSE



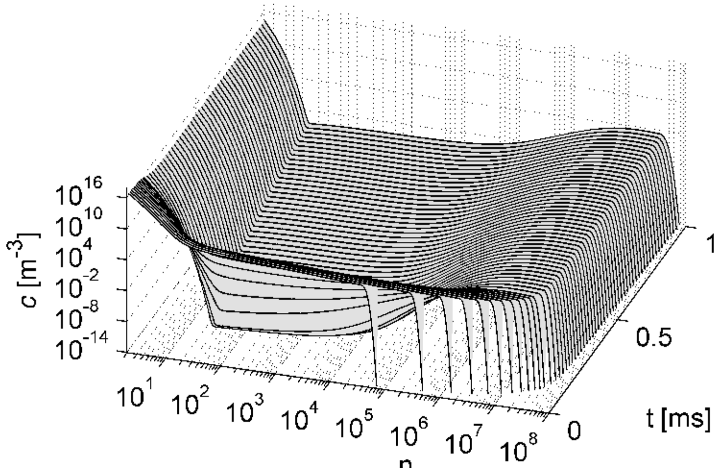
Droplet size distribution
t = 20, 40, 60, 80, 100 μs



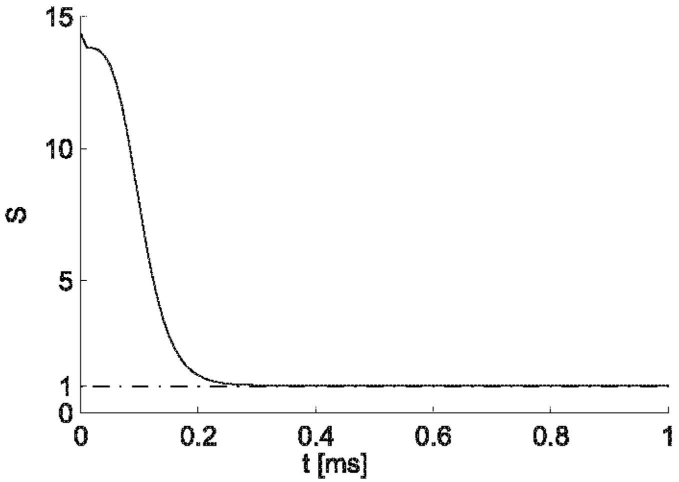
Supersaturaton S

- For long times depletion *cannot* be neglected
- Supersaturation S decreases and n_{cr} increases

RESULTS: WITH DEPLETION
TEST CASE: NUCLEATION PULSE



Droplet size distribution
t = 20, 40, 60, 80, 100 μs

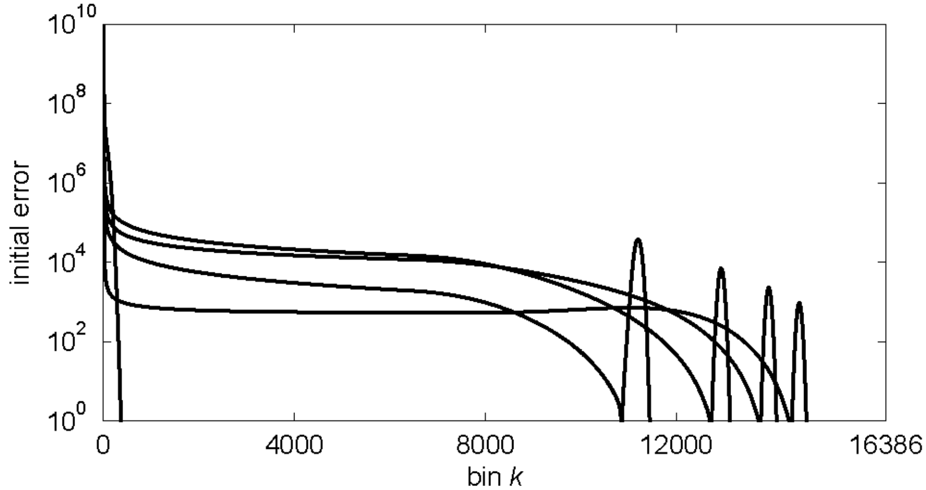


Supersaturaton S

- After 0.3 ms saturated conditions are reached

RESULTS: WITH DEPLETION
TEST CASE: NUCLEATION PULSE

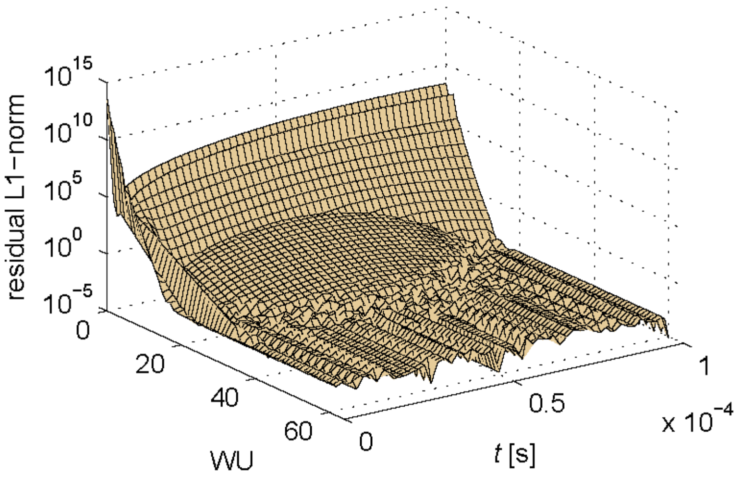
- Binned KE: initial error at different time steps



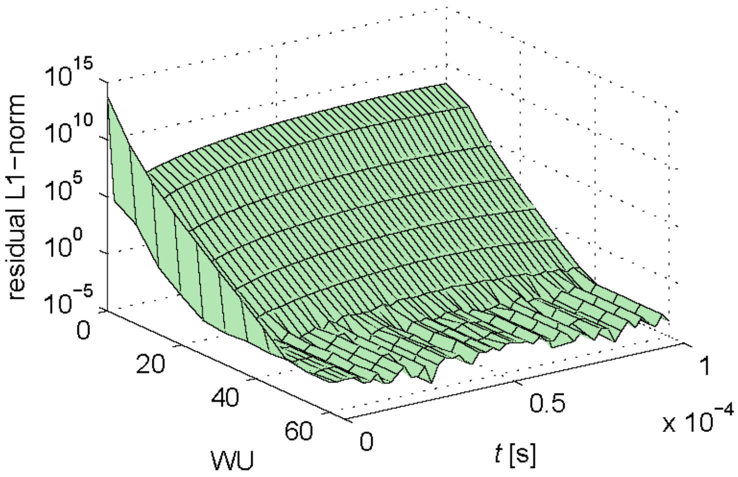
- Initial error contains more low frequency components
- Multi-level method is expected to benefit

RESULTS: WITH DEPLETION
TEST CASE: NUCLEATION PULSE

- Binned KE: Interior residual reduction



Relaxation

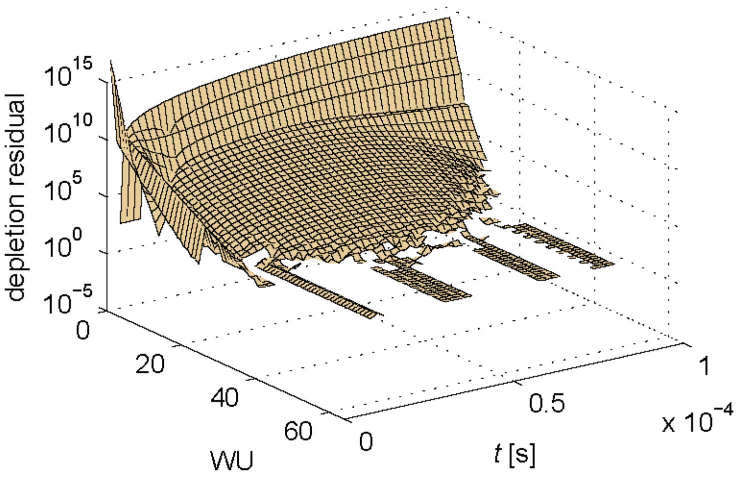


Multi-level cycles

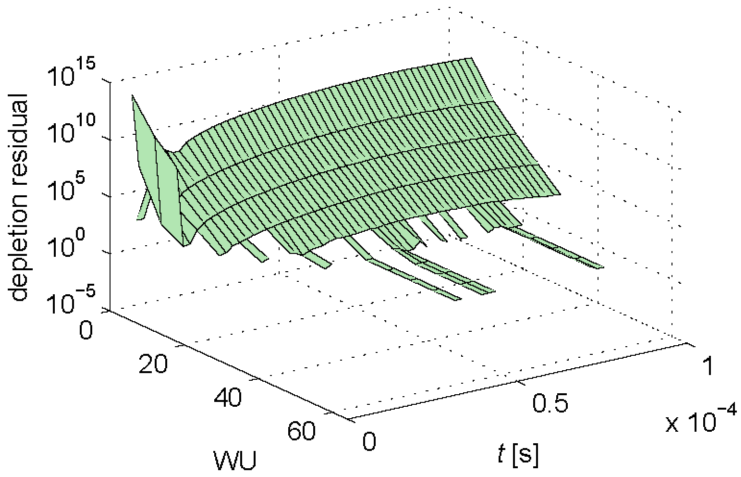
- Relaxation suffers from low frequency components
- <u>Multi-level less efficient</u>

RESULTS: WITH DEPLETION
TEST CASE: NUCLEATION PULSE

- Reason: Reduction of depletion equation



Relaxation



Multi-level cycles

- Relaxation applies global constraint more often
- Multi-level performance is stalled

CONCLUSIONS & RECOMMENDATIONS

- Introduction
- Theory
- Test case: Nucleation pulse
- Conclusions & recommendations

CONCLUSIONS

CONCLUSIONS & RECOMMENDATIONS

- Multi-level method is successfully applied to the KE
- Suitable coarsening has been devised which can represent the KE on different grids
- Applicable to multi-component condensation problems

RECOMMENDATIONS

- Investigate high-order time integration schemes
- Global constraint stalls coarse grid correction process
- Investigate non-uniform coarsening
  - Geometric
  - Algebraic MultiGrid (AMG)

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THANK YOU FOR YOUR ATTENTION