Emerging Models and Technologies for Multi-scale Modeling and Simulations of Nanostructured Material Formations and Property Predictions

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Outline

1. Introduction
2. Mathematical model in Macro-scale
3. Mathematical model in Micro-scale
4. Molecular dynamics simulations in atomic scale
5. Coupling

1. Introduction

Challenges in modeling Nanomaterial formation

- Occur at multiple time and length scales
- Need multidisciplinary knowledge
- Whole scale simulation relies on computing capacity
- Multiscale modeling is a good method to solve this problem

1. Introduction

Crystallization process

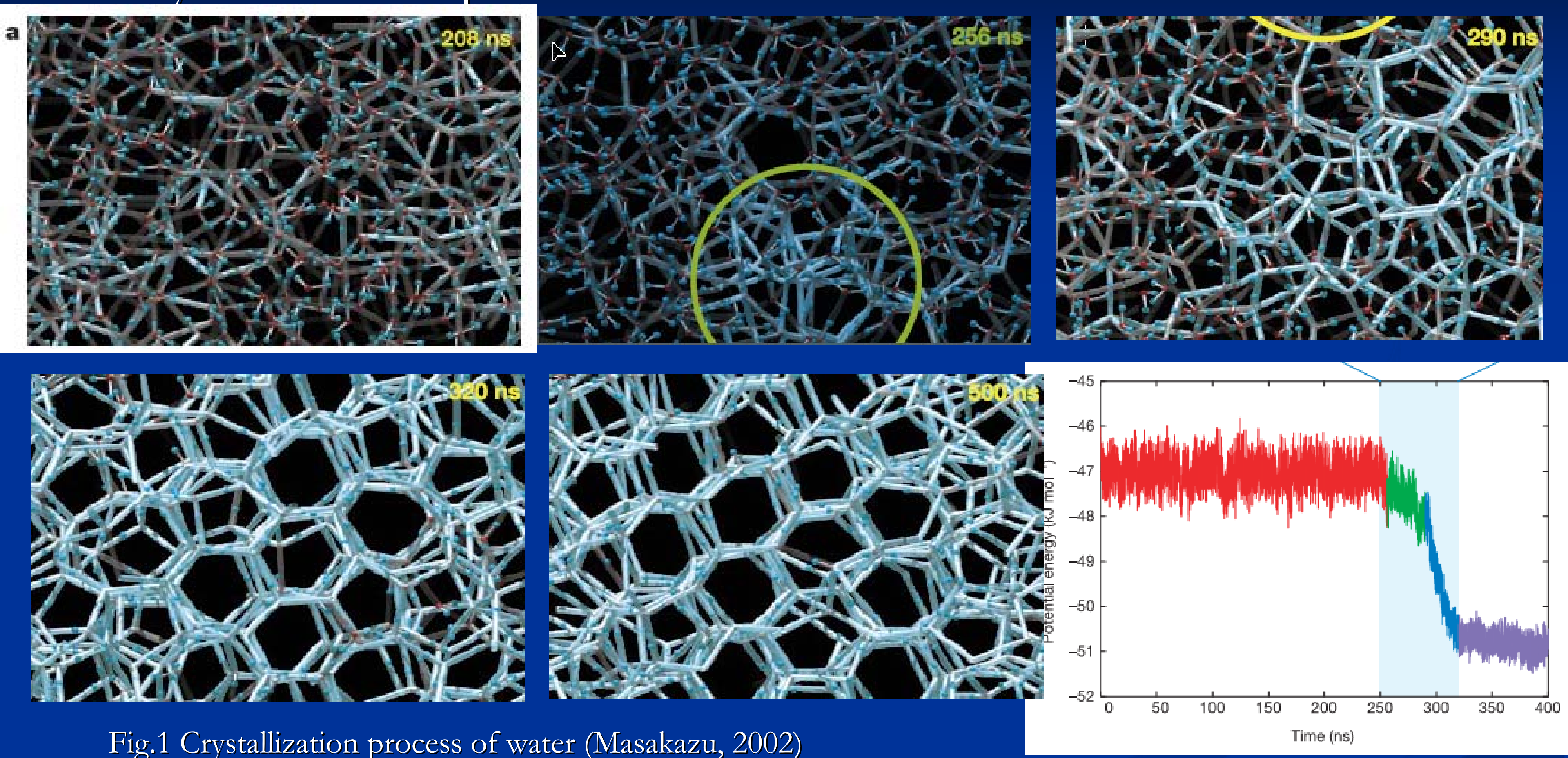


Fig.1 Crystallization process of water (Masakazu, 2002)

1. Introduction

Multiscale simulation

- Set up sub-model for different scale
- Couple sub-models
- Conduct whole-scale simulations on large-scale computing systems

2. Mathematical model in Macro-scale

Model is set up by finite element method with variable time step front tracking method to

$$([K]^n + [K]^{n+1} + \frac{2}{\Delta t}([C]^n + [C]^{n+1}))\{T\}^{n+1} = (\frac{2}{\Delta t}([C]^n + [C]^{n+1}) - [K]^n - [K]^{n+1})\{T\}^n \quad (1)$$

at time=t^n, $[K]^n, [C]^n, \{T\}^n, \xi^n, \dot{\xi}^n$ is known

$$\dot{\xi}^n = \frac{1}{\rho\lambda}[k_s[\frac{\partial N_i}{\partial x}]\{T_i\}_s - k_l[\frac{\partial N_i}{\partial x}]\{T_i\}_l]^n \quad (2)$$

2. Mathematical model in Macro-scale

At time= t^{n+1}, $[K]^{n+1}$,$[C]^{n+1}$ is known, use (1) and (2) to obtain temperature distribution at time t^{n+1}

$$\{T\}_r^{n+1} = \frac{(\frac{2}{\Delta t_0}\{[C]^n + [C]^{n+1}\} - [K]^n - [K]^{n+1})\{T\}^n}{(\frac{2}{\Delta t_0}\{[C]^n + [C]^{n+1}\} + [K]^n + [K]^{n+1})}$$

Where, r is iteration number

2. Mathematical model in Macro-scale

Numerical Test

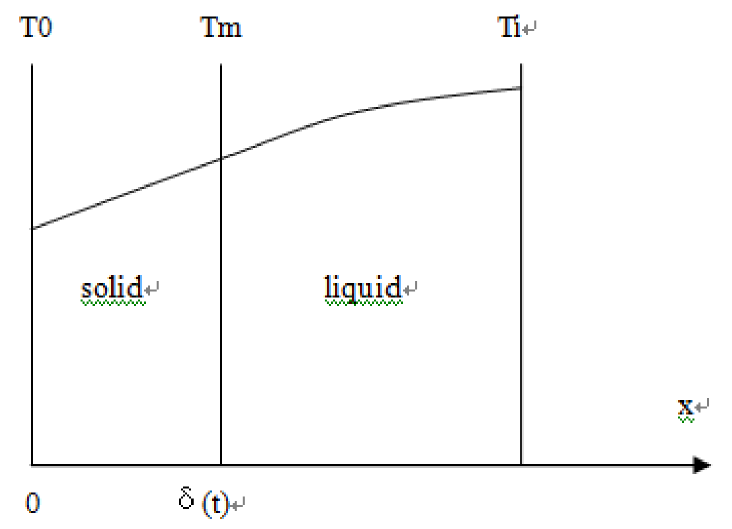


Fig.1 One-dimensional phase change problem

2. Mathematical model in Macro-scale

Numerical Experiments

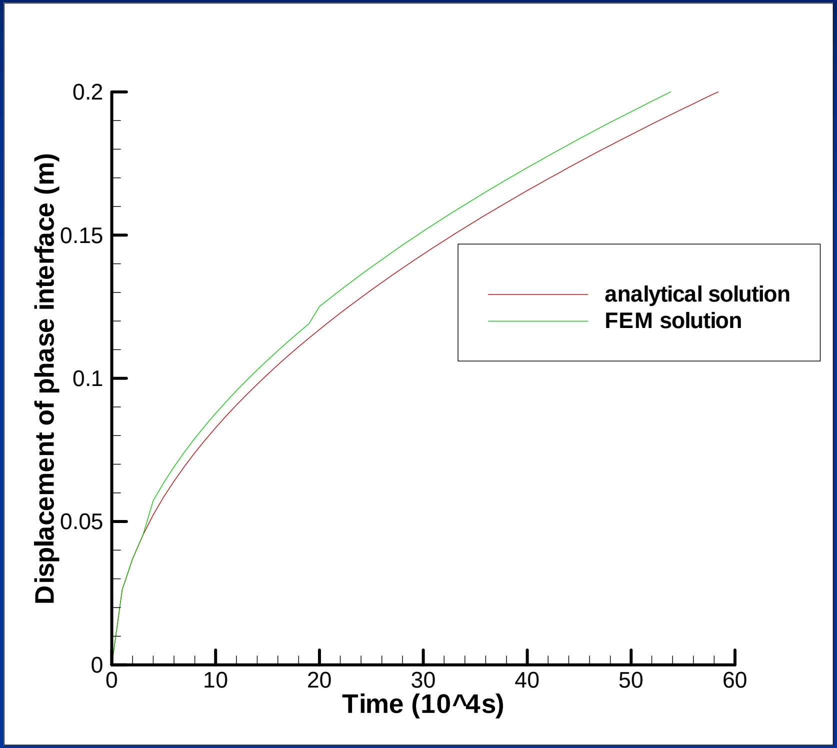


Fig.2 Phase interface position

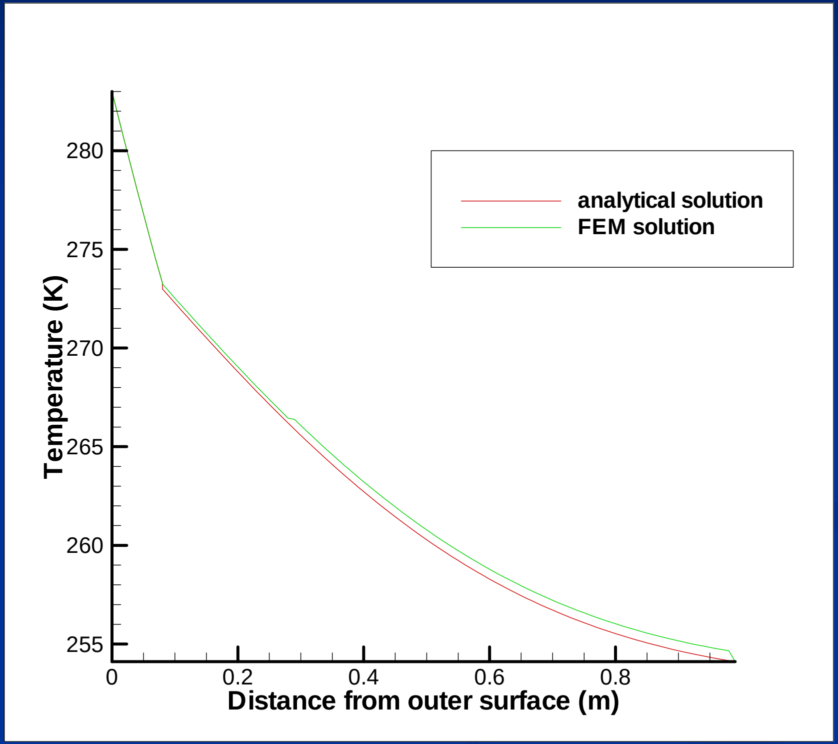


Fig.3 Temperature distribution

3. Mathematical model in Micro-scale

The thermal wave model is used in micro-scale.

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

where: τ is mean free time, mathematically,

$$\tau = I/v_s$$

where: l is the effective mean free path

v_s is the speed of sound

3. Mathematical model in Micro-scale

Numerical Experiments

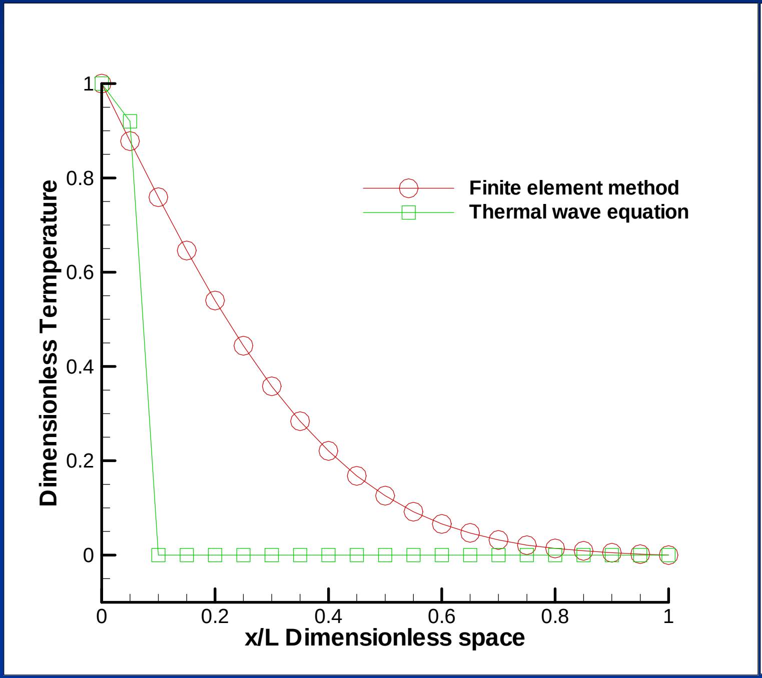


Fig.4 Temperature profiles at t=0.1

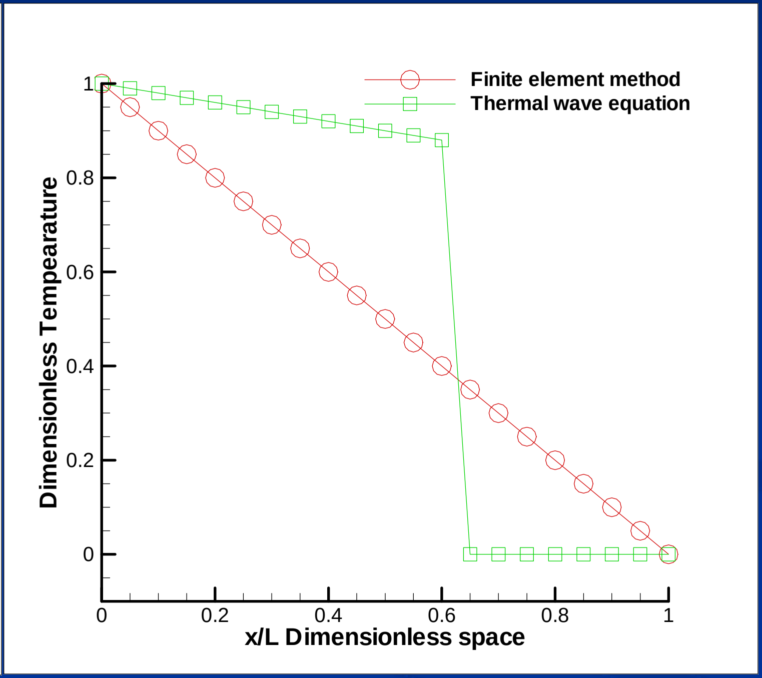


Fig.5 Temperature profiles at t=1

3. Mathematical model in Micro-scale

Numerical Test

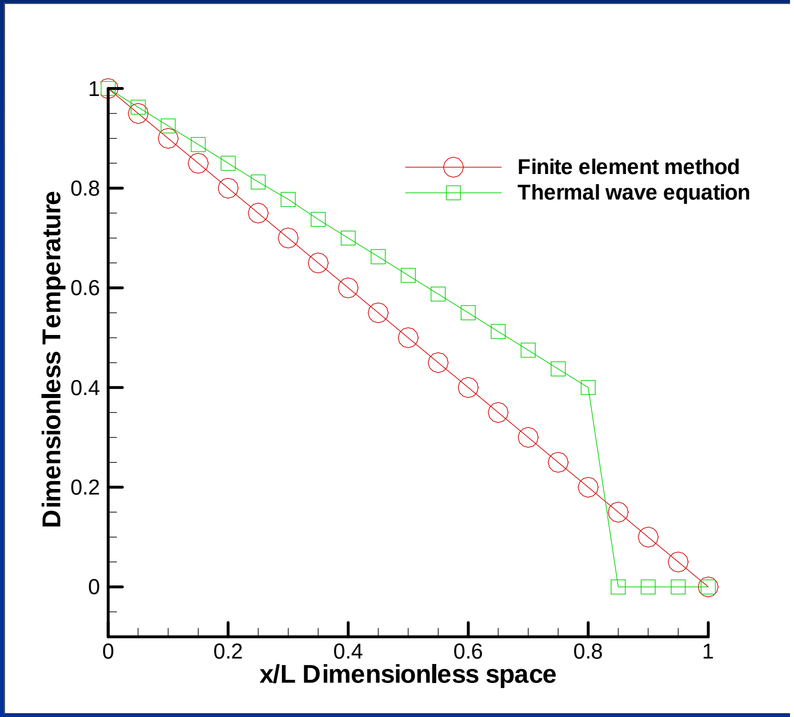


Fig.6 Temperature profiles at t=1.5

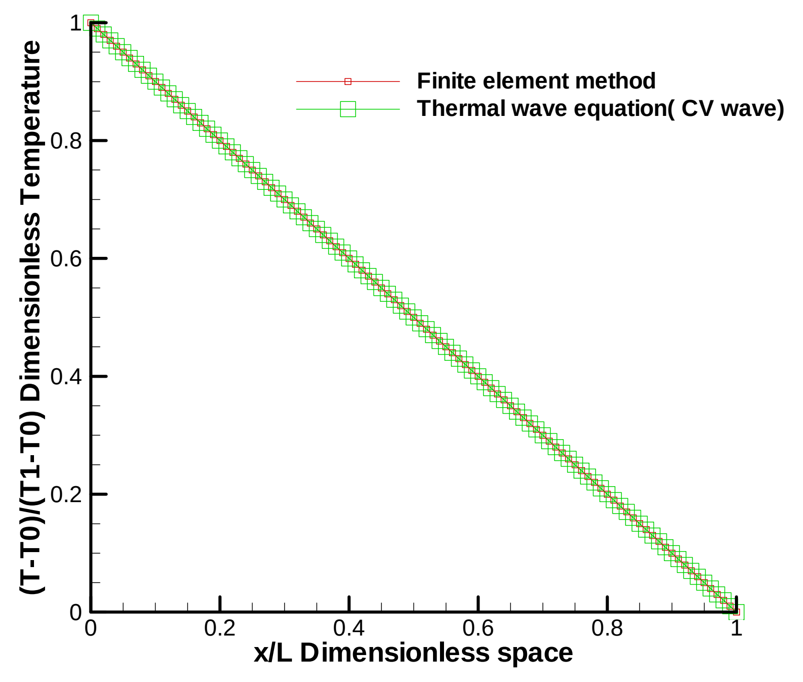


Fig.7 Temperature profiles at steady state

4. Molecular dynamics simulation in atomic scale

- Perform molecular dynamics simulation to simulate ice melting
- NPT ensemble
- 1 atmosphere, Temperature is 310K
- Different configurations are performed

4. Molecular dynamics simulation in atomic scale

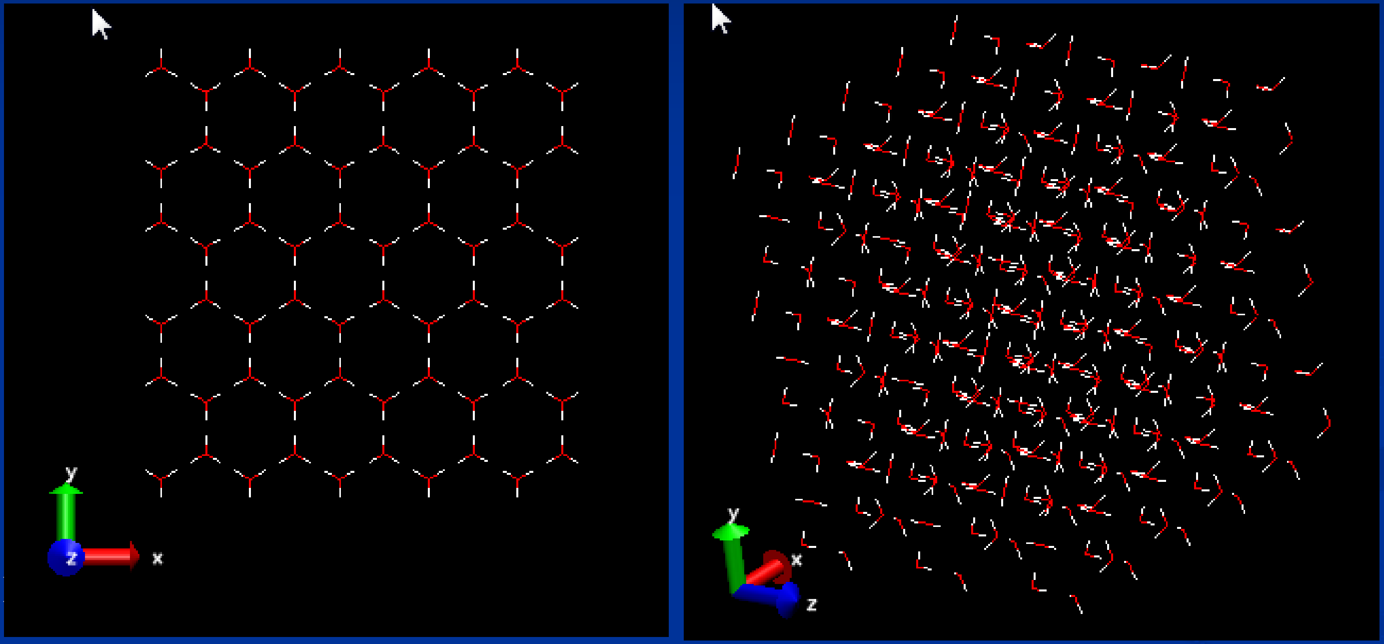


Fig.8

4. Molecular dynamics simulation in atomic scale

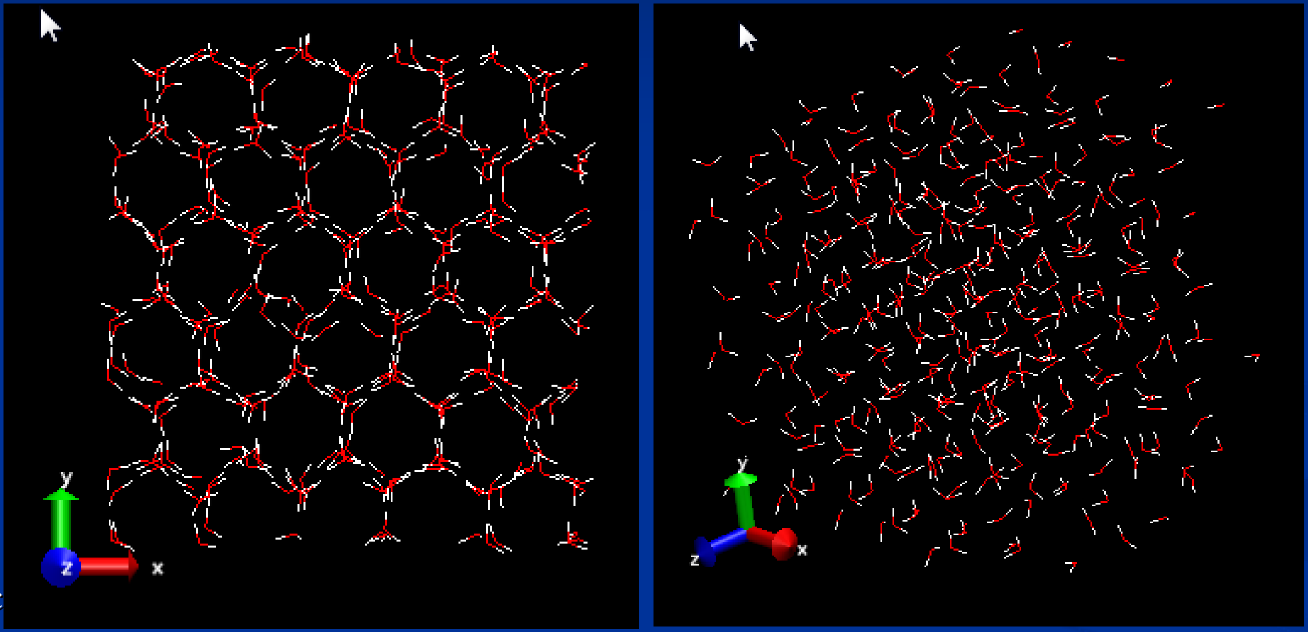


Fig.9 Ic

4. Molecular dynamics simulation in atomic scale

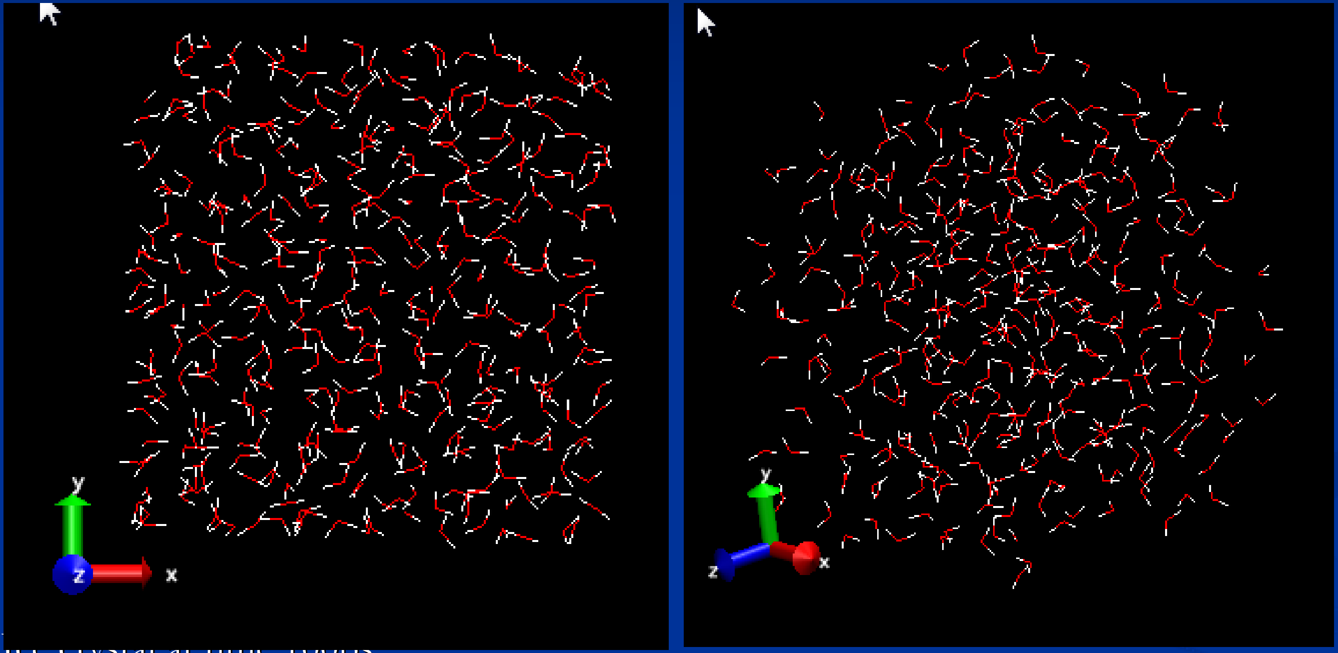
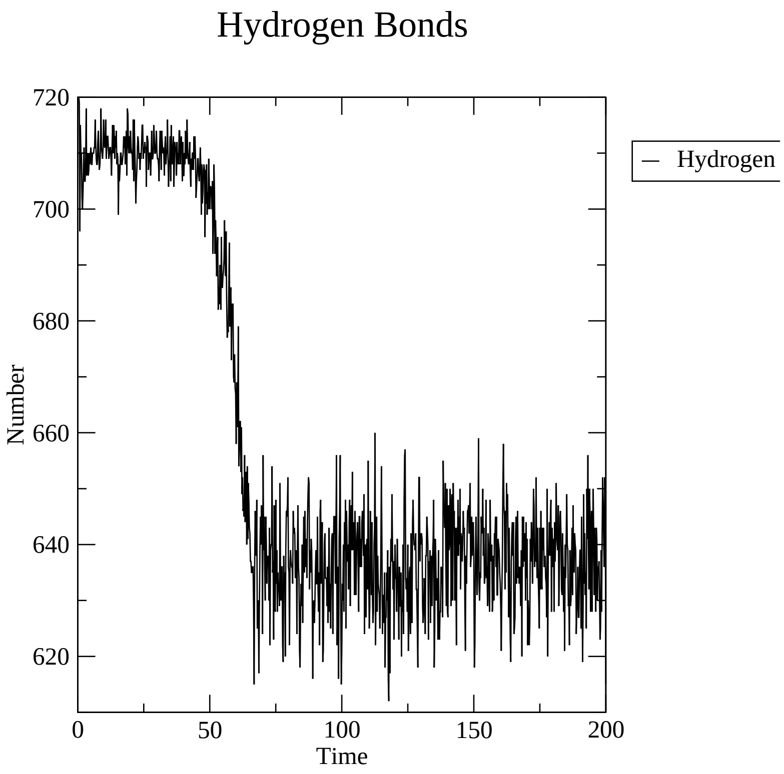
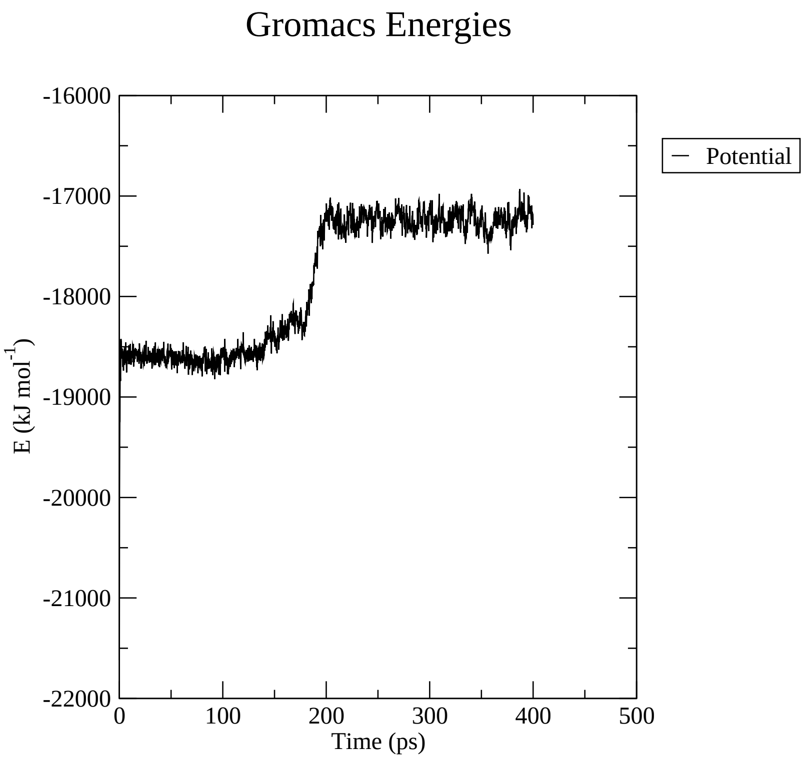


Fig.10 Ice crystal at time 100ps

4. Molecular dynamics simulation in atomic scale





4. Molecular dynamics simulation in atomic scale

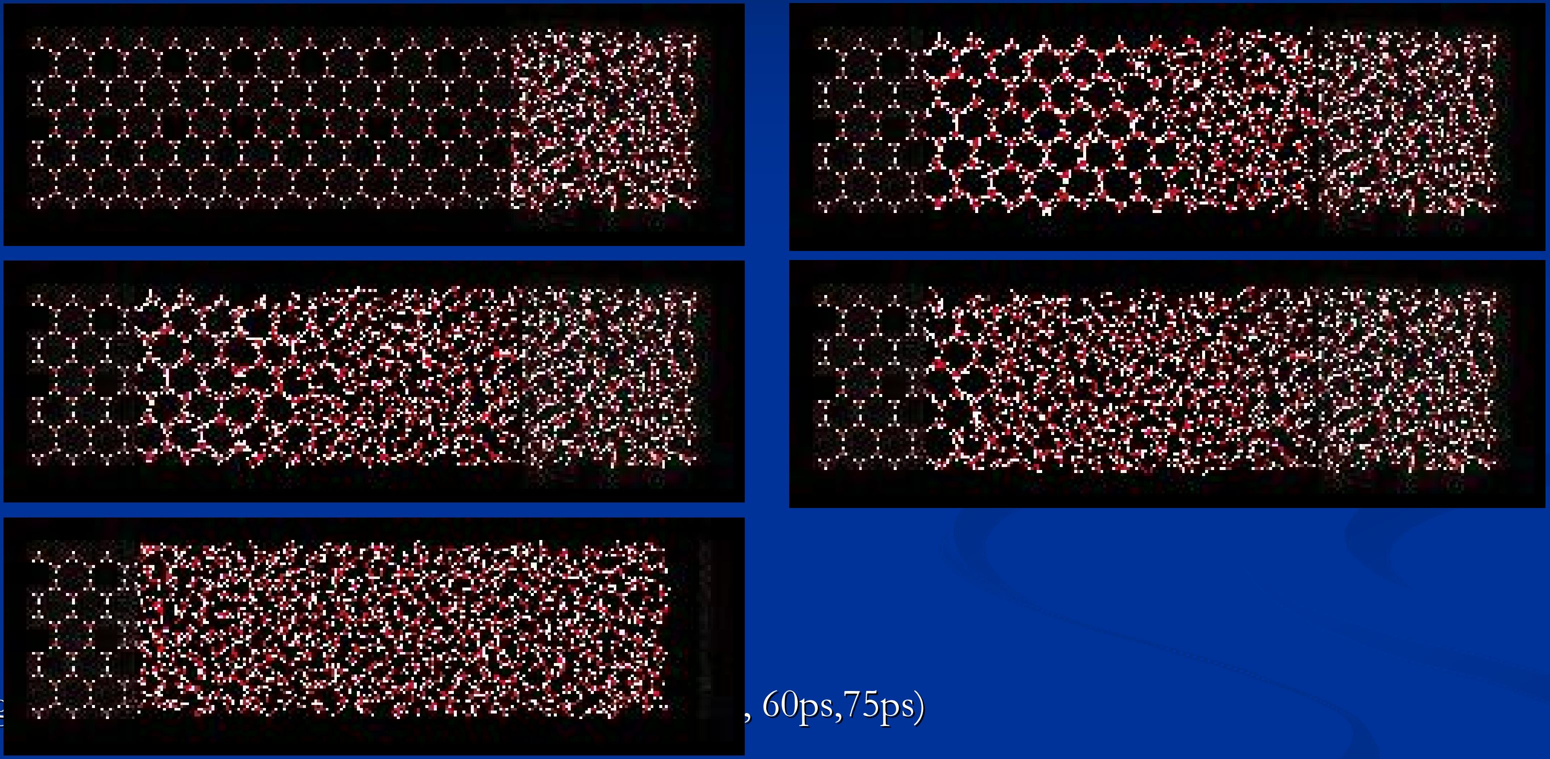


Fig , 60ps,75ps)

5. Coupling

- Using Parallel Bridging Domain Multiscale method (PBDM) to couple each sub model together.
- PBDM--- decomposing the physical domain into different computational domains each of which can be processed in parallel
- Coupling will be done in following work

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Thanks and Question?