A Multi-scale Model for Simulations of Crystallization/Solidification in the Formation of Nano-structured Materials on Large-scale Parallel Computing System

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Outline

- Complex Transport Phenomena
- Previous Mathematical Models
  - Continuum Model (1980s)
  - Micro-macroscopic Model (1990s)
- Total atomic-micro-meso-macro model
- Cyberinfrastructure enabled resources
- Large-scale HPC and DIC

Complex Transport Phenomena

- Mass, heat (energy), momentum transports
- Transfer mechanisms:
  - Cystalization, diffusive, convective, etc.
- status described by physical characteristic properties (scalar variables)
- processes described by physical processing properties (vector variables)

Complex Transport Phenomena

- Classification
  - medium: three phases (gas, liquid, and solid) or the mixed combination
  - fluid flow
  - multiphase flow (liquid and solid)
    - flow in porous medium
    - fluidized-bed flow and flow packed-bed
    - dispersed and suspended flow
    - with phase change
    - with multi-components

Complex Transport Phenomena

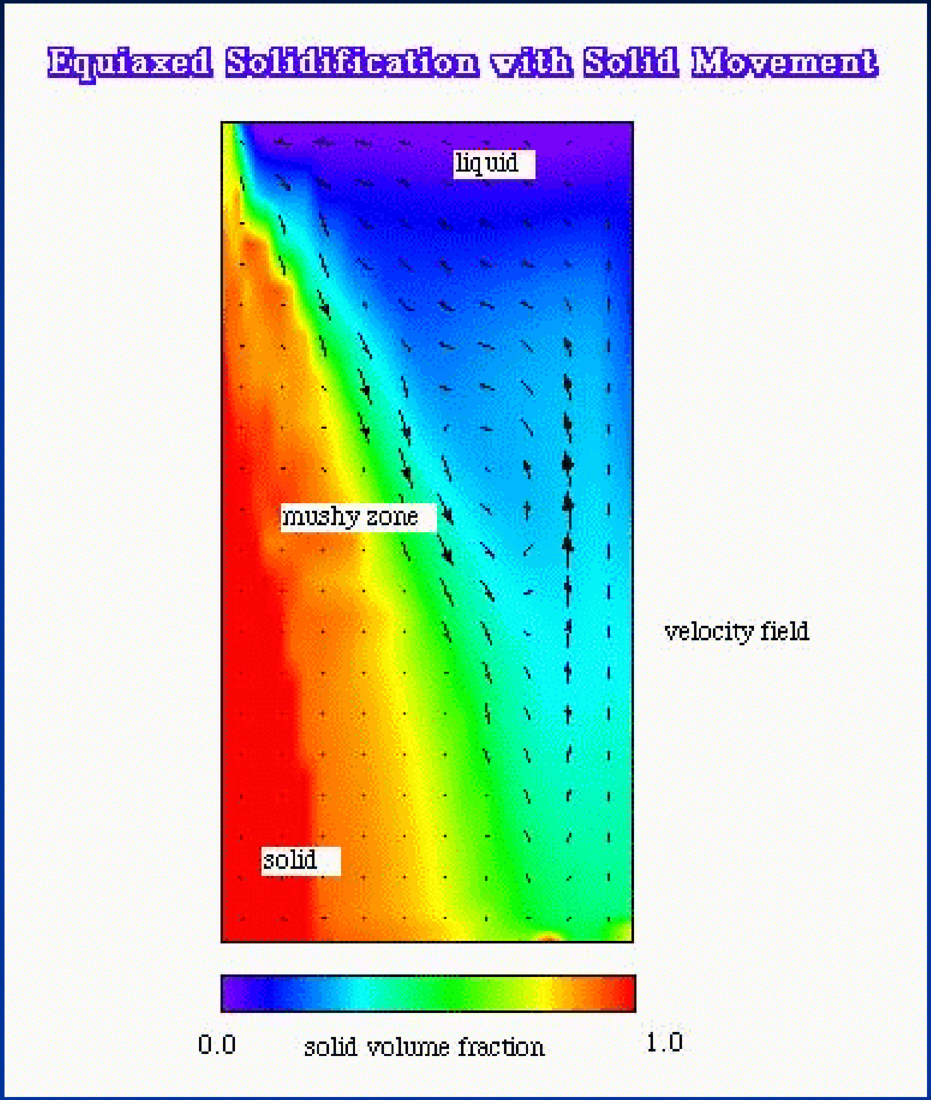
- Solidification and Crystallization
  - Multi-components
  - Binary systems
  - Atomic level, nucleation, crystal growth and formation, packaging and fluidization, sedimentation, …final patterns and properties.
- Heat and species driving forces

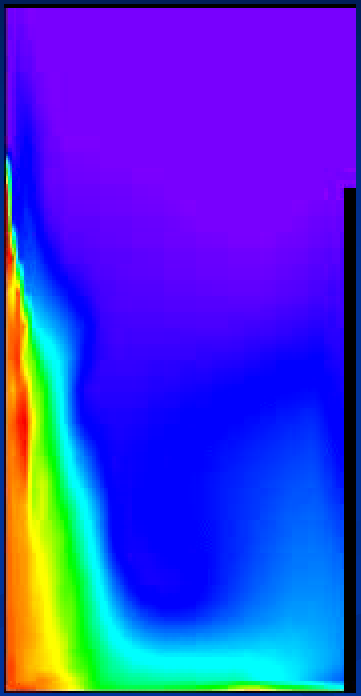
Previous Models

- Driving forces from previous modeling and simulations
  - Solidification process of metal alloys (nucleation, multi-scale)
  - Mechanical Cracking (media discontinuity, domain mapping)

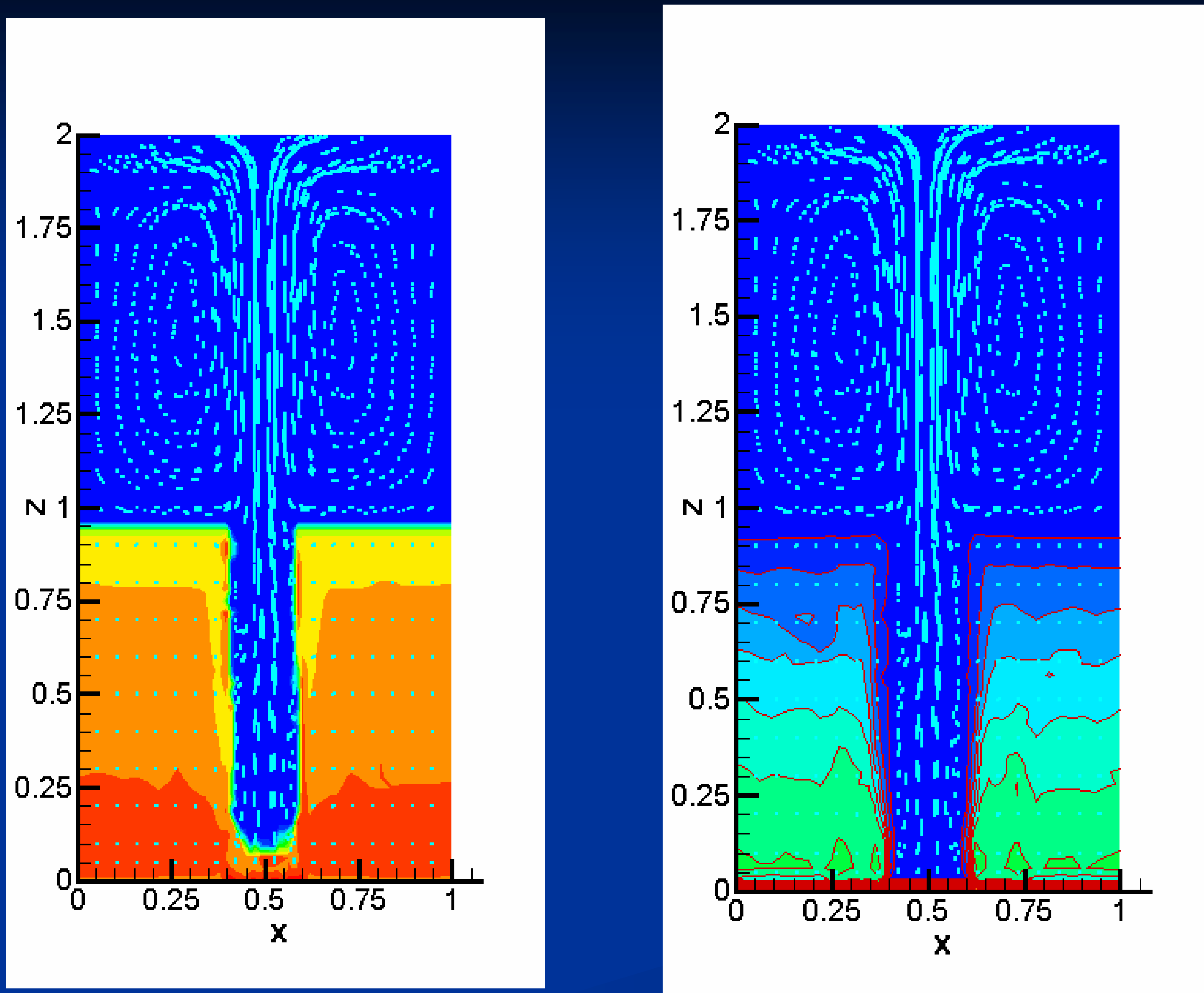
Art-of-Arts in Current Model

- Flow around dendritic crystals (using phase-field method)
- Flow around growing crystals (using phase-field method)
- Flow around 3D crystals (using phase field method)

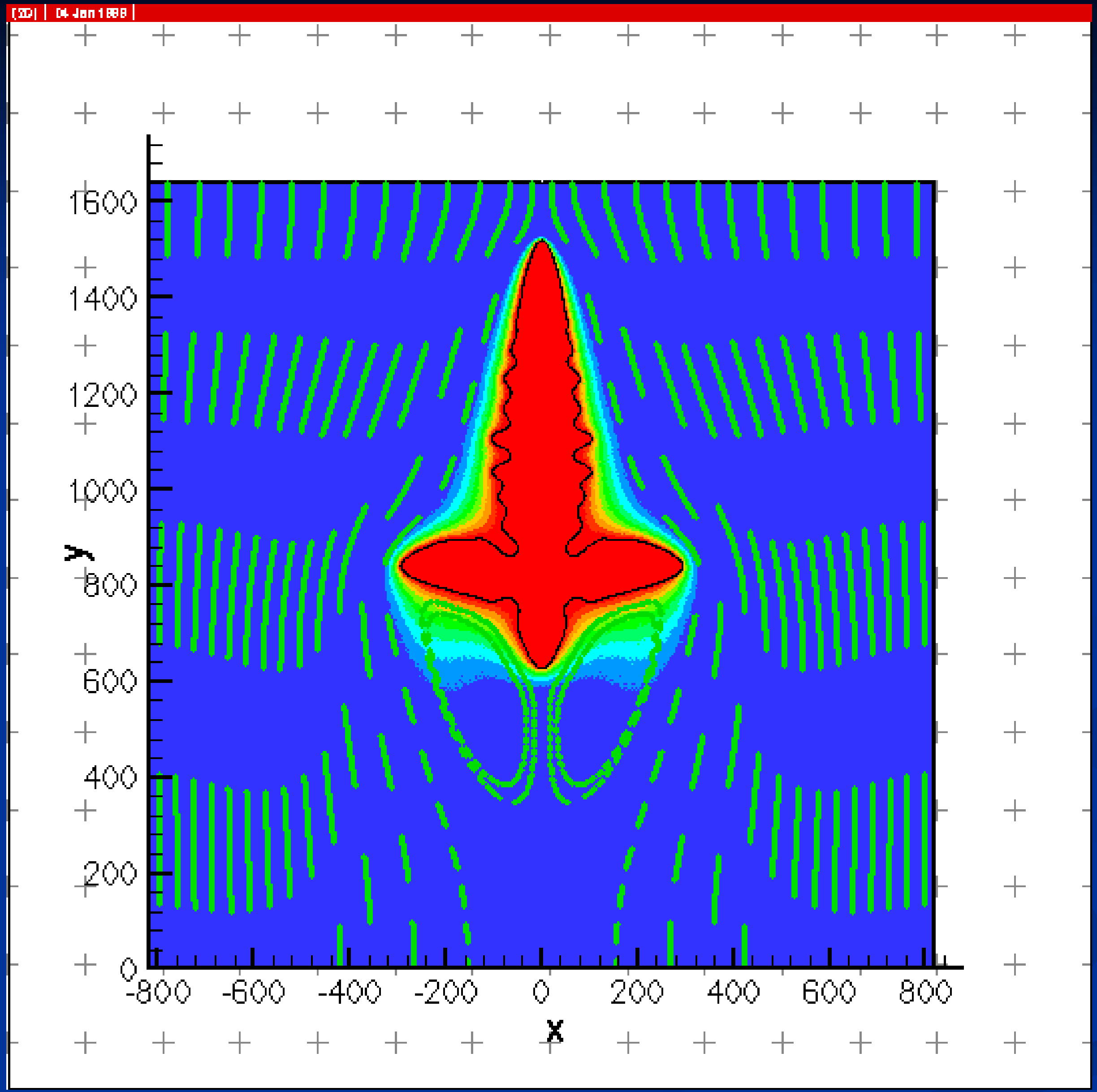




Ni and Beckermann, 1994



C. Beckermann's research work (UI)



C. Beckermann's research work (UI)

Mathematical Modeling

- Mathematical approaches
  - microscopic description
  - macroscopic description
    - mixture model (continue model)
    - volume averaging technique
    - macroscopic model
    - macro/microscopic model
    - macro/micro/atomic model

Mathematical Modeling

- Volume averaging technique
  - definition

$$< \Psi_k > = \frac{1}{V_o}\int_{V_k} X_k \Psi_k dV = \varepsilon_k < \Psi_k >^k = \frac{\varepsilon_k}{V_k}\int_{V_k} X_k \Psi_k dV$$

$$\overline{\Psi}_{ki} = \frac{1}{A_i}\int_{A_i} \Psi_k dV$$

$$\varepsilon_k = \frac{V_k}{V_o}$$

$$\sum_k \varepsilon_k = 1$$

Mathematical Modeling

- Volume averaging technique

$$< \frac{\partial \Psi_k}{\partial t} > = \frac{\partial < \Psi_k >}{\partial t} - \frac{1}{V_o}\int_{A_k} \Psi_k w_k n_k \, dA$$

$$< \nabla \Psi_k > = \nabla < \Psi_k > + \frac{1}{V_o}\int_{A_k} \Psi_k n_k \, dA$$

$$< \nabla \Psi_k > = \varepsilon_k \nabla < \Psi_k >^k + \frac{1}{V_o}\int_{A_k} \tilde{\Psi}_k n_k \, dA$$

$$\tilde{\Psi}_k = (\Psi_k - < \Psi_k >^k) X_k$$

Mathematical Modeling

- Physical considerations
  - mass conservation
  - momentum conservation
  - heat/energy conservation
  - species conservation
  - entropy irreversibility (new)

Mathematical Modeling

- Microscopic mass conservation

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k v_k) = 0$$

- Macroscopic mass conservation

$$\frac{\partial}{\partial t}(\varepsilon_k \rho_k) + \nabla \cdot (\varepsilon_k \rho_k < v_k >^k) = \Gamma_k = -\frac{1}{V_o}\int_{A_k} \rho_k (v_k - v_k) \cdot n_k dA$$

Mathematical Modeling

- Microscopic momentum conservation

$$\frac{\partial}{\partial t}(\rho_k v_k) + \nabla \cdot (\rho_k v_k v_k) = -\nabla p_k + \nabla \cdot \tau_k + b_k$$

Mathematical Modeling

- Macroscopic momentum conservation

$$\frac{\partial}{\partial t}(\varepsilon_k \rho_k < v_k >^k) + \nabla \cdot (\varepsilon_k \rho_k < v_k >^k < v_k >^k) =$$

$$-\nabla(\varepsilon_k < p_k >^k) + \nabla \cdot (< \tau_k > + < \tau_k^t >)$$

$$+ M_k^\Gamma + M_k^d + \varepsilon_k < b_k >^k$$

Mathematical Modeling

- where

$$M_k^{\Gamma} = -\frac{1}{V_o}\int_{A_k} \rho_k v_k (v_k - v_k)\cdot n_k dA = \overline{v_{ki}}\Gamma_k$$

$$M_k^{d} = \frac{1}{V_o}\int_{A_k} (\tau_k - p_k I)\cdot n_k dA$$

Mathematical Modeling

- where

$$< \tau_k > = \mu_k^* \{ \nabla (\varepsilon_k < v_k >^k + [\nabla (\varepsilon_k < v_k >^k]^t$$
$$- < v_s >^s \nabla \varepsilon_k - \nabla \varepsilon_k < v_s >^s \}$$

Mathematical Modeling

- Microscopic energy conservation

$$\frac{\partial}{\partial t}(\rho_k h_k) + \nabla \cdot (\rho_k h_k v_k) = -\nabla \cdot q_k + g_k$$

Mathematical Modeling

- Macroscopic energy conservation

$$\frac{\partial}{\partial t}(\varepsilon_k \rho_k < h_k >^k) + \nabla \cdot (\varepsilon_k \rho_k < h_k >^k < v_k >^k) =$$
$$\nabla (< q_k > + < q_k^t >) + Q_k^{\Gamma} + Q_k^q + \varepsilon_k < g_k >^k$$

$$< q_k > = -k_k^* \cdot \varepsilon_k \nabla < T_k >^k$$

$$< q_k^t > = - < \rho_k h'_k v'_k >$$

Mathematical Modeling

- where

$$Q_k^{\Gamma} = -\frac{1}{V_o}\int_{A_k} \rho_k h_k (v_k - v_k)\cdot n_k dA = \overline{h_{ki}}\Gamma_k$$

$$Q_k^{q} = -\frac{1}{V_o}\int_{A_k} q_k \cdot n_k dA$$

Mathematical Modeling

- Microscopic species conservation

$$\frac{\partial}{\partial t}(\rho_k C_k) + \nabla \cdot (\rho_k C_k v_k) = -\nabla \cdot j_k + r_k$$

Mathematical Modeling

- Macroscopic species conservation

$$\frac{\partial}{\partial t}(\varepsilon_k \rho_k < C_k >^k) + \nabla \cdot (\varepsilon_k \rho_k < C_k >^k < v_k >^k) =$$
$$\nabla(< j_k > + < j^t_k >) + J^{\Gamma}_k + J^q_k + \varepsilon_k < r_k >^k$$

$$< j_k > = -D^*_k \cdot \rho_k \varepsilon_k \nabla < C_k >^k$$

$$< j^t_k > = - < \rho_k C_k v_k >$$

Mathematical Modeling

- where

$$J_k^{\Gamma} = -\frac{1}{V_o}\int_{A_k} \rho_k C_k (v_k - v_k) \cdot n_k dA = \overline{C_{ki}}\Gamma_k$$

$$J_k^{j} = -\frac{1}{V_o}\int_{A_k} j_k \cdot n_k dA$$

Mathematical Modeling

- Interfacial balances

$$\sum_k \Gamma_k = 0$$

$$\sum_k (M_k^{\Gamma} + M_k^{\tau}) + M_i = 0$$

$$\sum_k (Q_k^{\Gamma} + Q_k^{q}) + Q_i = 0$$

$$\sum_k (J_k^{\Gamma} + J_k^{j}) + J_i = 0$$

Mathematical Modeling

- Thermodynamic relations
  - interfacial relation

$$T_{ki} = T_i$$

$$\frac{C_{ki}}{C_{li}} = f(T_i^{k-l})$$

$$C_{li} = g(T_i)$$

$$(k \neq l)$$

Mathematical Modeling

- Thermodynamic relations
  - enthalpies and density relation

$$<h_k>^k = f^q(<T_k>^k, <C_k>^k)$$

$$<\rho_k>^k = f^\rho(<T_k>^k, <C_k>^k)$$

Mathematical Modeling

- Macroscopic Flex Modeling
  - Interfacial stresses

$$M_k^{\tau} = +\overline{p_{ki}} \nabla \varepsilon_k + M_k^d$$

$$M_k^d = -\frac{1}{V_o} \frac{1}{2} \rho_l A_d C_D \,|< v_s >^s - < v_s >^s| (< v_l >^l - < v_l >^l)$$

$$M_k^d = -\varepsilon_l^2 \mu_l K^{(2)^{-1}} (< v_l >^l - < v_l >^l)$$

$$M_i = \frac{1}{V_o} \int_{A_i} \sigma \zeta n_s dA = -\sigma \overline{\zeta} \nabla \varepsilon_s$$

$$M_k^{\Gamma} = \overline{v_{ki}} \Gamma_k$$

Mathematical Modeling

- Macroscopic Flex Modeling
  - Interfacial heat flex

$$Q_k^q = \frac{A_i}{V_o}\frac{k_k}{l_k^q}(\overline{T_i} - \langle T_k \rangle^k)$$

$$Q_k^\Gamma = \overline{H_{ki}}\Gamma_k$$

Mathematical Modeling

- Macroscopic Flex Modeling
  - Interfacial species flex

$$J_k^j = \frac{A_i}{V_o}\frac{D_k}{l_k^j}(\overline{C_i} - < C_k >^k)$$

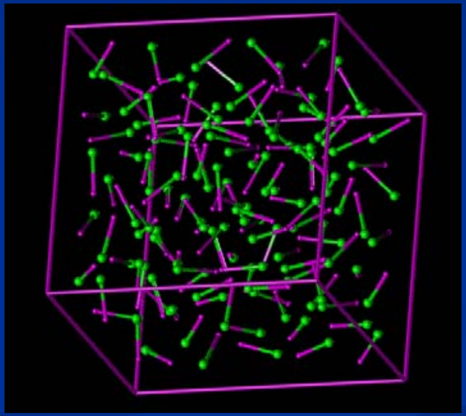
$$J_k^\Gamma = \overline{C_{ki}}\Gamma_k$$

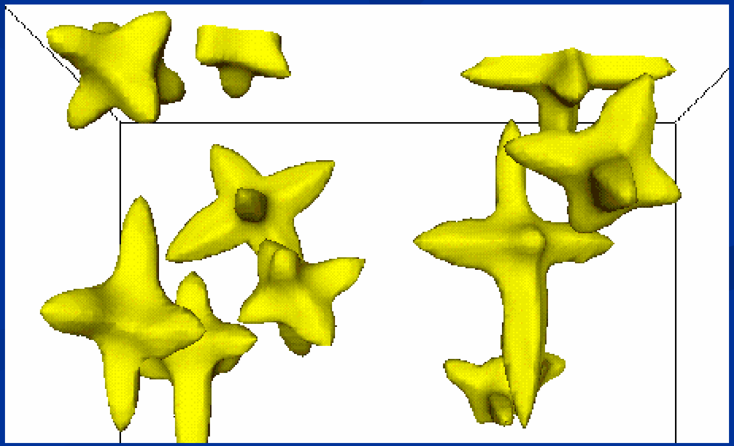
Applications

- Metal Casting and foundry in Metallurgy
- Physics
- Chemical engineering
- Materials processing
- Automobile industrials
- Geological science and geophysics
- Reology
- Mineralogy
- Cryobiology

Micro-macroscopic coupling

- Molecular dynamics simulation for modeling nucleation
- Molecular dynamics for crystal growth and kinetics
- Hierarchical model and concurrent model



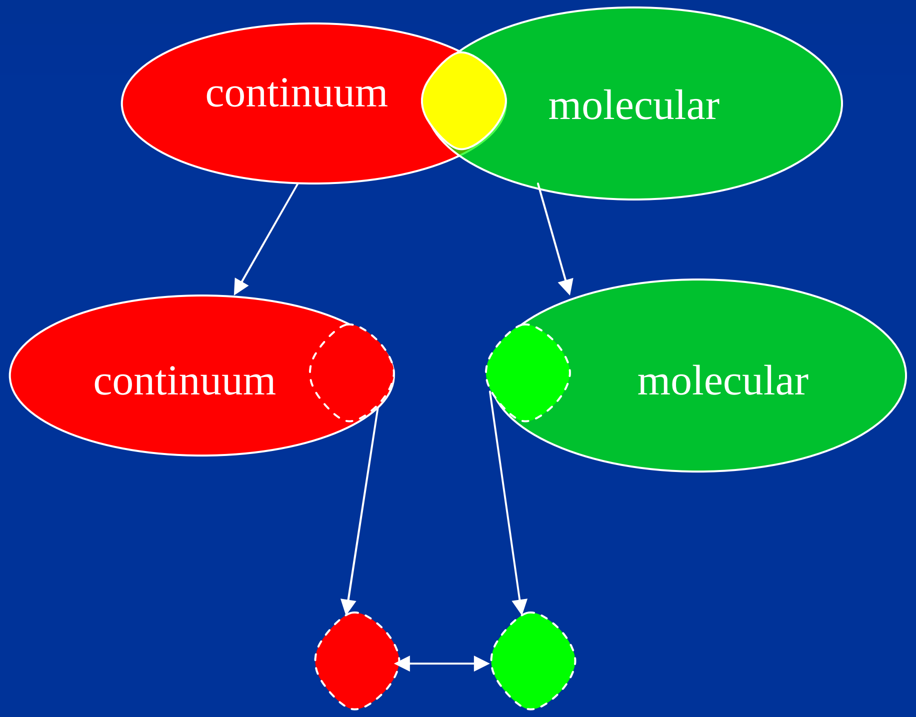


Micro-macroscopic coupling

- Nanocrystal generation, formation, and growth
- Nano-particples
- Molecular modeling for Interfacial phenomena, particle collision, and interaction
- Composite nanoparticle imposing and impingement
- Compose nano-materials property predictions (chemical, physical and mechanical)

Grid-based Bridging Domain Multiscale

- **High-performance computing:**
  - The bridging domain coupling method is one of the best candidates which can be extended as a high-performance computing enhanced multiscale method



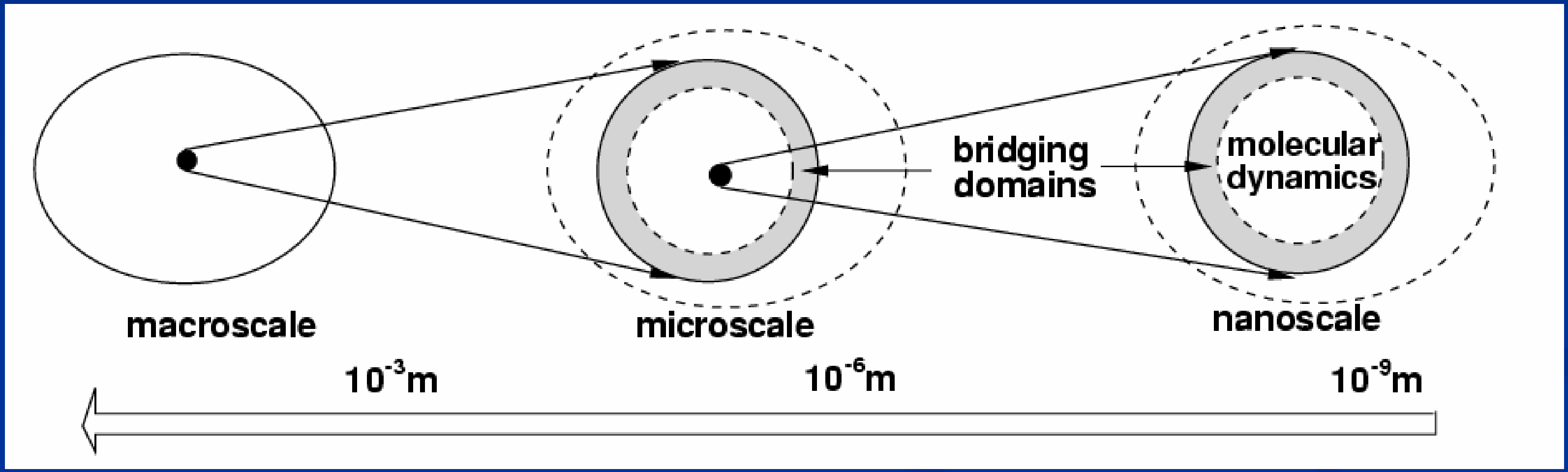
A bridging domain coupling model

At each time step, equations of motion are solved separately in each domain for nodal/atomic velocities

Then, nodal/atomic velocities in the bridging domain are corrected

Grid-based Bridging Domain Multiscale

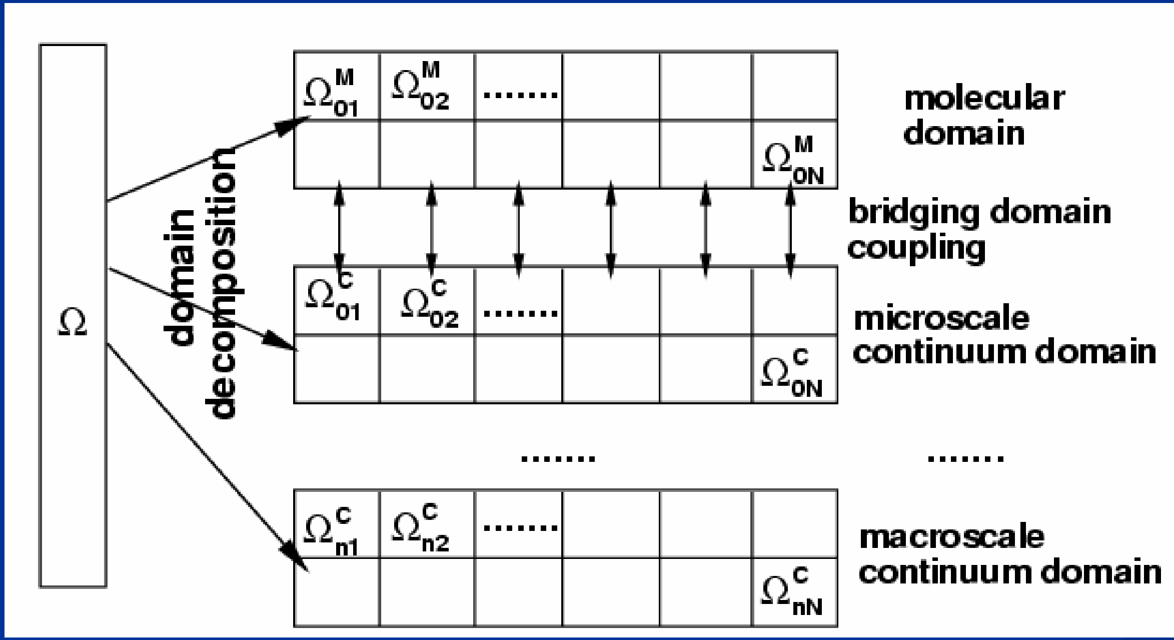
- **Grid-based bridging domain multiscale method:**
  - Multiple-length-scale model



Macroscale: Linear finite element methods
Microscale: Meshfree particle methods
Nanoscale: Molecular dynamics

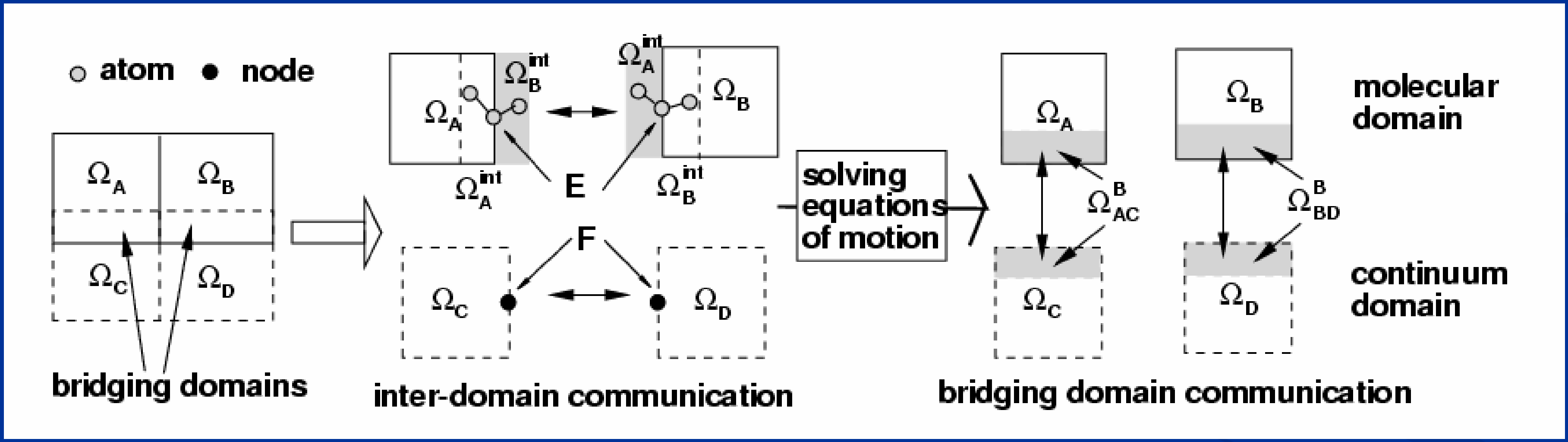
Grid-based Bridging Domain Multiscale

- **Grid-based bridging domain multiscale method:**
  - Domain Decomposition

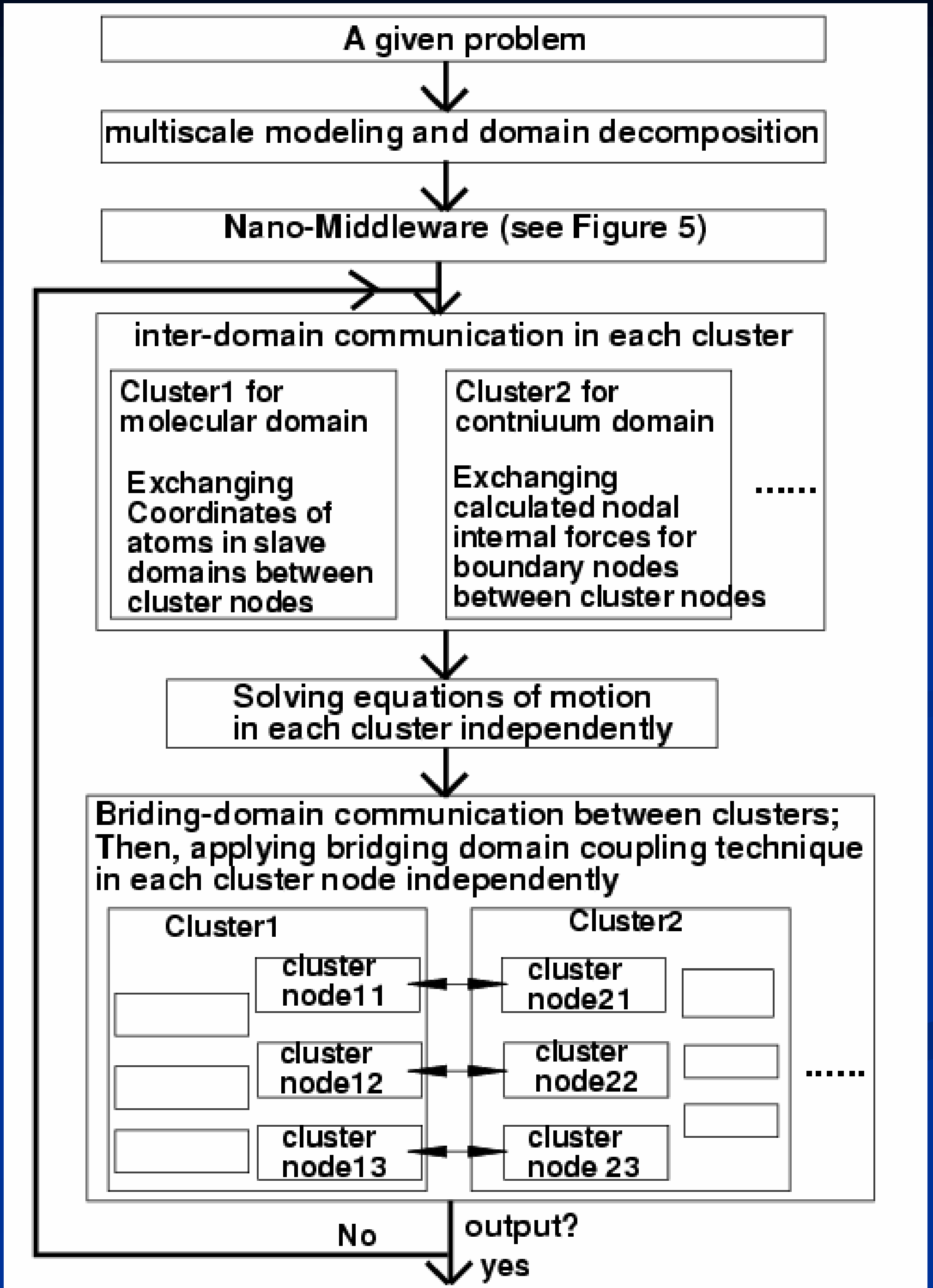


Grid-based Bridging Domain Multiscale

- **Grid-based bridging domain multiscale method:**
  - Domain Communication



- Grid-based bridging domain coupling multiscale method:
  - Flow chart
  - Workflow



Conclusion

- Most numerical methods in nanotechnology have limitations on length/time scales.
- Innovative thinking is needed to re-engineering both modeling and simulations
- Intensive computations are needed due to
  - Tons of repeated numerical tests.
  - Modeling large nano systems.
- Cyber-enabled resources and solutions for above issues.
- Integration of multiscale methods and higher performance computing in nanotechnology

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