Understanding Information Mediation Issues in Multiscale Design

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Increasing energy use

Increasing impact on the environment

Increasing resource scarcity

Energy and environmental challenges

innovation

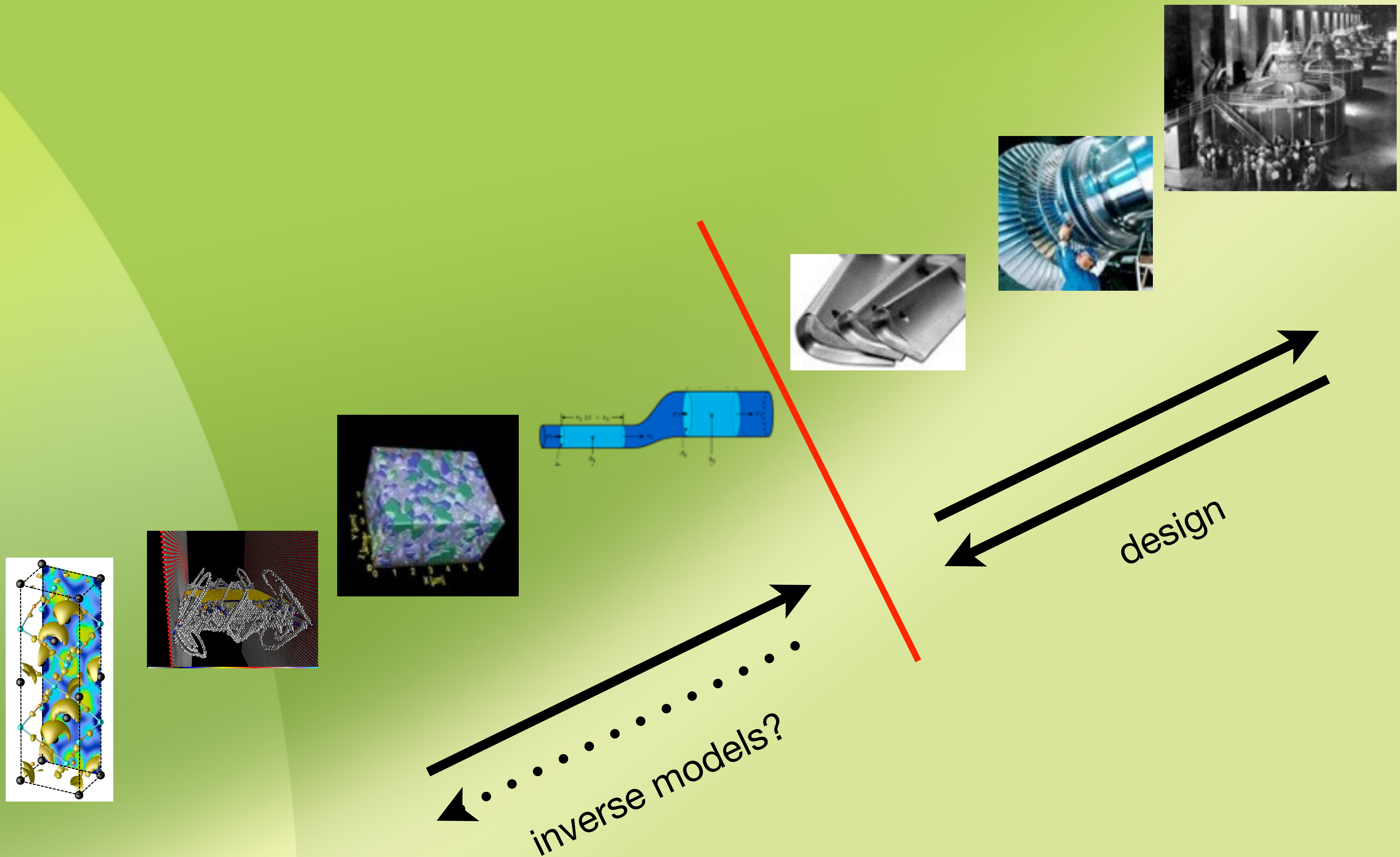
decision making

engineering

...

actionable information
that changes something

Why create models?



Design across scales

- models
- simulations
- databases
- sensors
- …

“models”

What's needed

Information

1. Integration
2. Mediation
3. Interaction

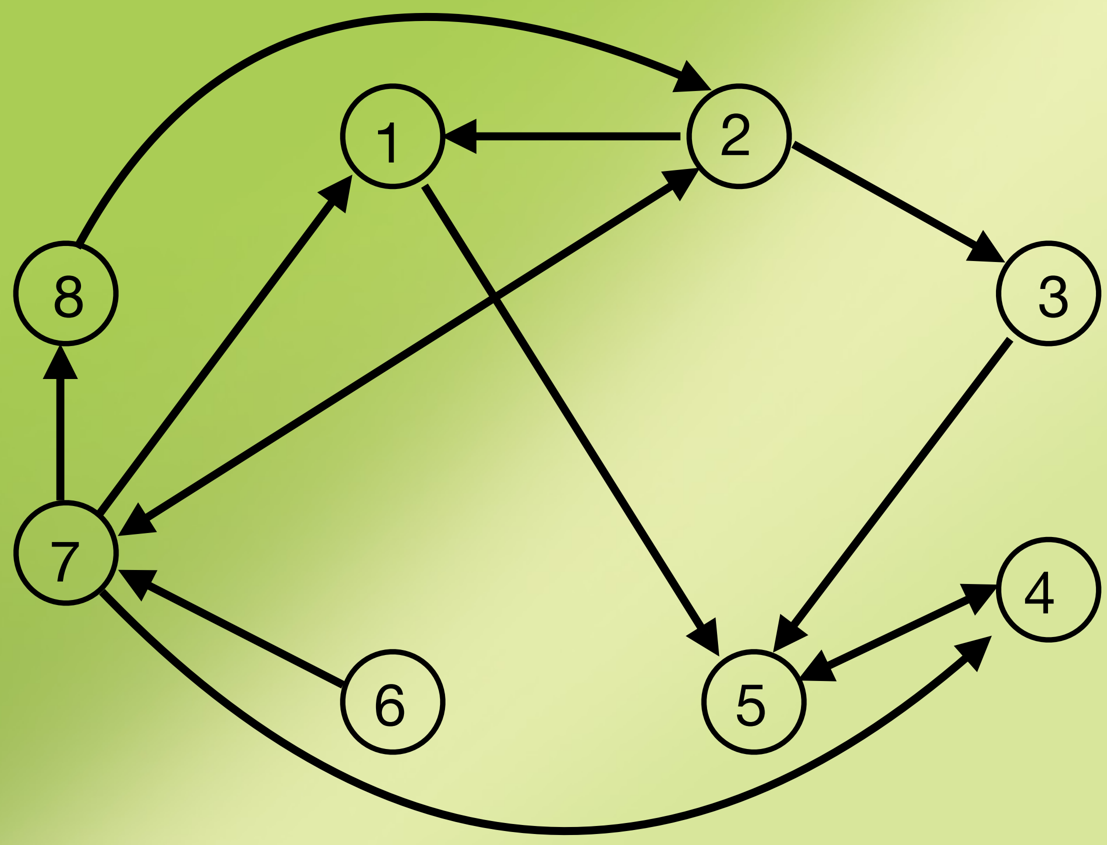
What's needed

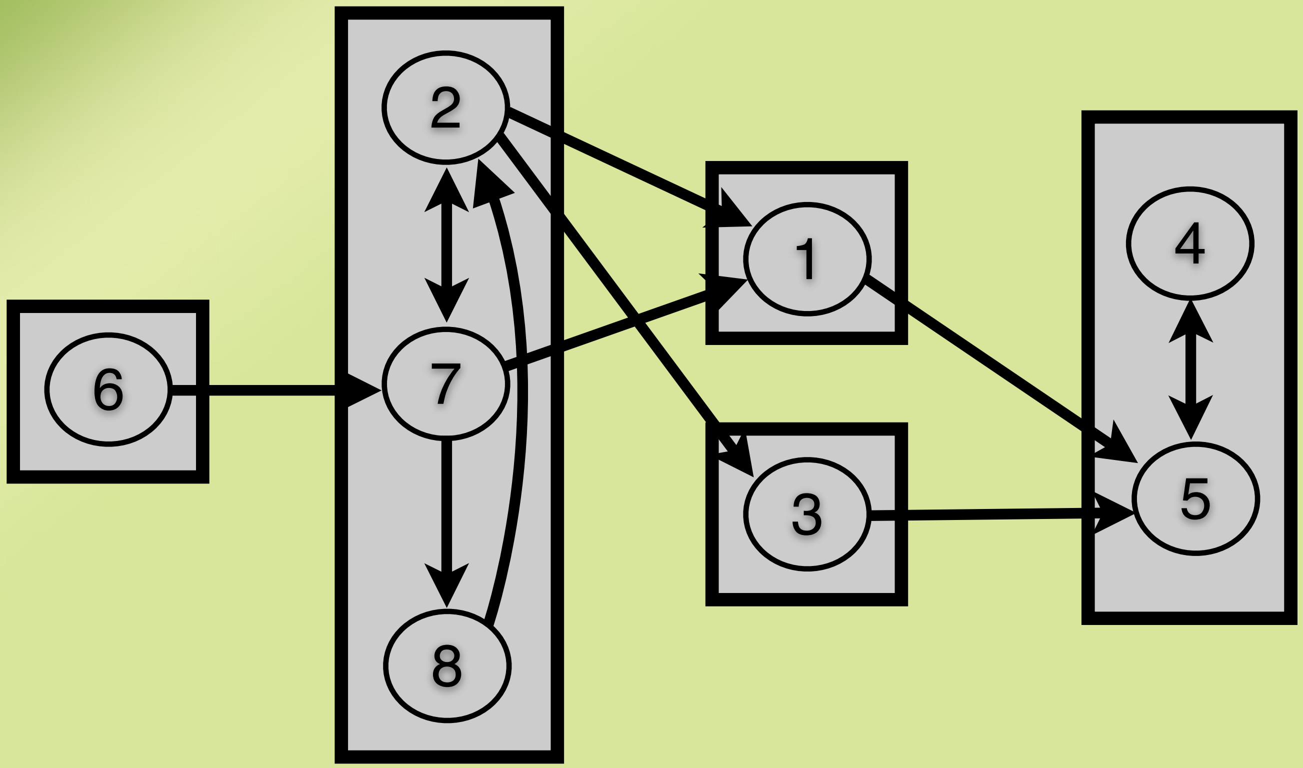
Information

1. Integration
2. Mediation
3. Interaction

- the development of the needed models
- the integration of these models to form federated model sets
- the establishment of a unified design environment based on the integrated model sets

- organize interconnected models to optimize solution





Organization of solutions

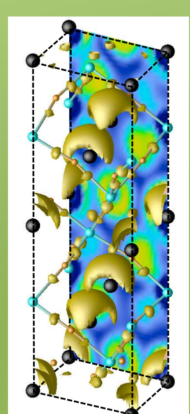
- **Constituency**
  the capability of models to come together in groups that have coherence and substitutability
- **Articulation**
  a simple and precise mechanism for describing how the models are chosen, linked, executed, and results reported
- **Convergence**
  a knowledge of the topological mapping of the federation and the capability to route and converge information through the federation to complete the assigned tasks

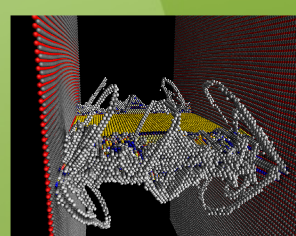
Federated model set requirements

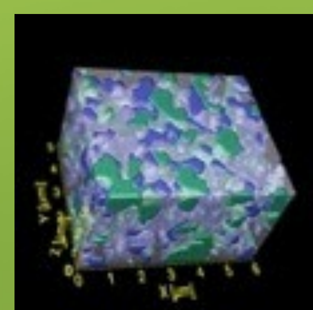
- enable models to couple together “on-the-fly” without intervention
- models must “know” whether they can link and what information that they require and deliver (identifiers)
- must be able to ensure that the information has the right units, attributes, …
- must be able to identify the *boundaries* that models need with other models

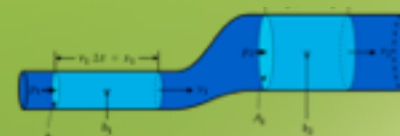
model to model communication

"information passing", in which information at one scale is passed as input to a larger scale









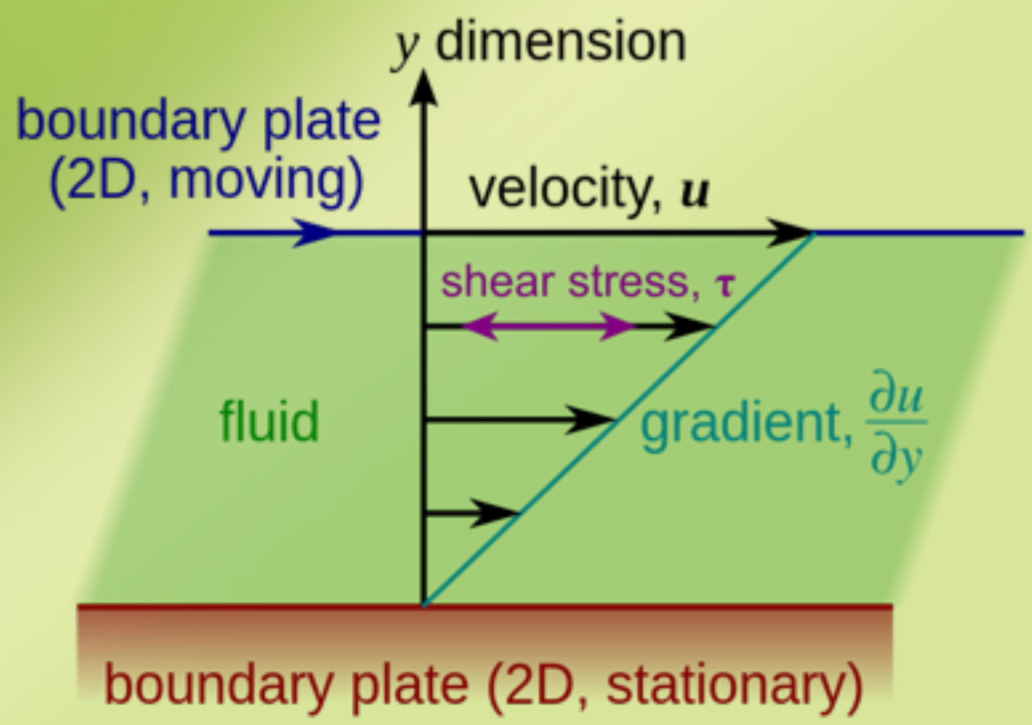
"concurrent multiscale", which is used when separation of scales is not possible or desirable

Multiple scales

Create a hybrid system (a “testbed”) to examine key aspects of information mediation for linked (concurrent) multiscale simulations

- information transfer between models
- boundaries between models
- convergence of the solution
- stability

- upper velocity is set as boundary condition
- examine atomistic-level effects of fluid/surface interactions (bottom boundary) on fluid flow



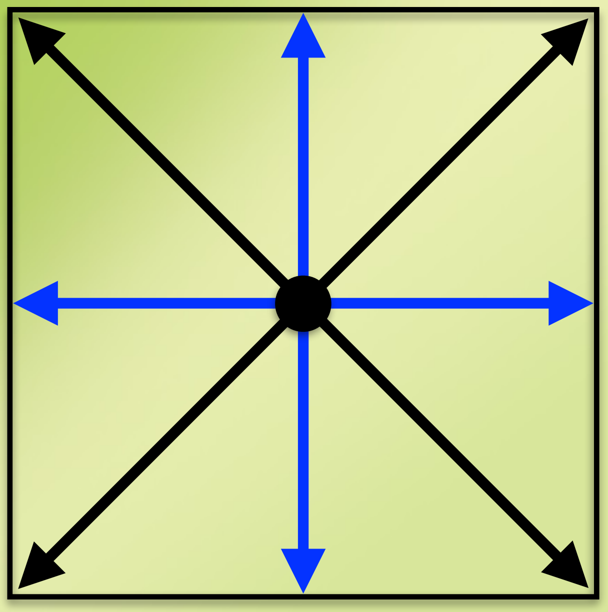
http://en.wikipedia.org/wiki/File:Laminar_shear.svg

Test problem: Couette flow

- Fluid flow simulations
  - Lattice Boltzmann method
  - lattice-based solution to Navier-Stokes equation
  - very useful for situations with complex boundary conditions

- Atomistic-level simulations
  - molecular dynamics

- single-particle distribution functions ($f_i(\vec{r},t)$) move along lattice sites

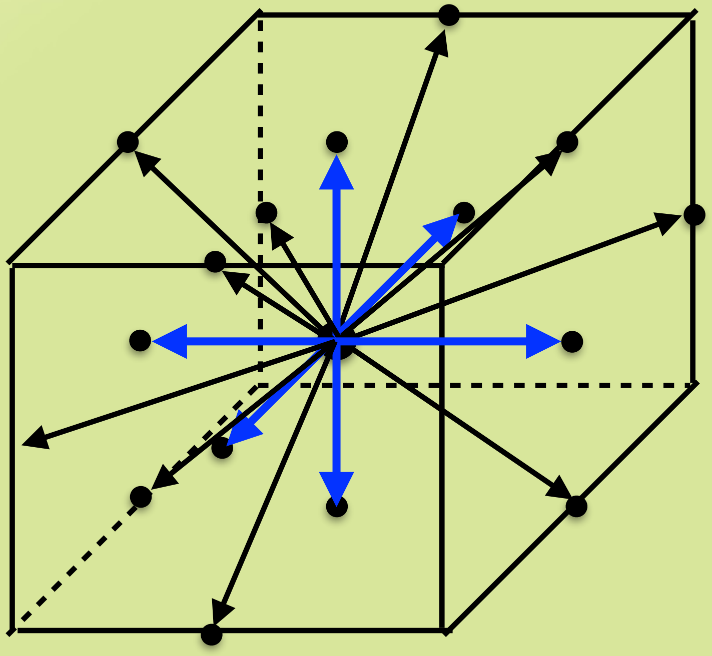


- dynamics

$$f_i\left(\vec{r}+\vec{v}_i\Delta t, t+\Delta t\right)=f_i\left(\vec{r},t\right)+\frac{\Delta t}{\tau}\left(f_i^{eq}\left(\vec{r},t\right)-f_i\left(\vec{r},t\right)\right)$$

- "collisions" lead to equilibrium distribution

$$f_i^{eq}\left(\vec{r},t\right)=w_i\rho\left(1+\frac{\vec{v}_i\cdot\vec{u}}{c_s^2}+\frac{\left(\vec{v}_i\cdot\vec{u}\right)^2}{2c_s^4}-\frac{u^2}{2c_s^2}\right)$$



- measurable quantities:

$$\rho=\sum_i f_i, \quad \rho\vec{u}=\sum_i \vec{v}_i f_i$$

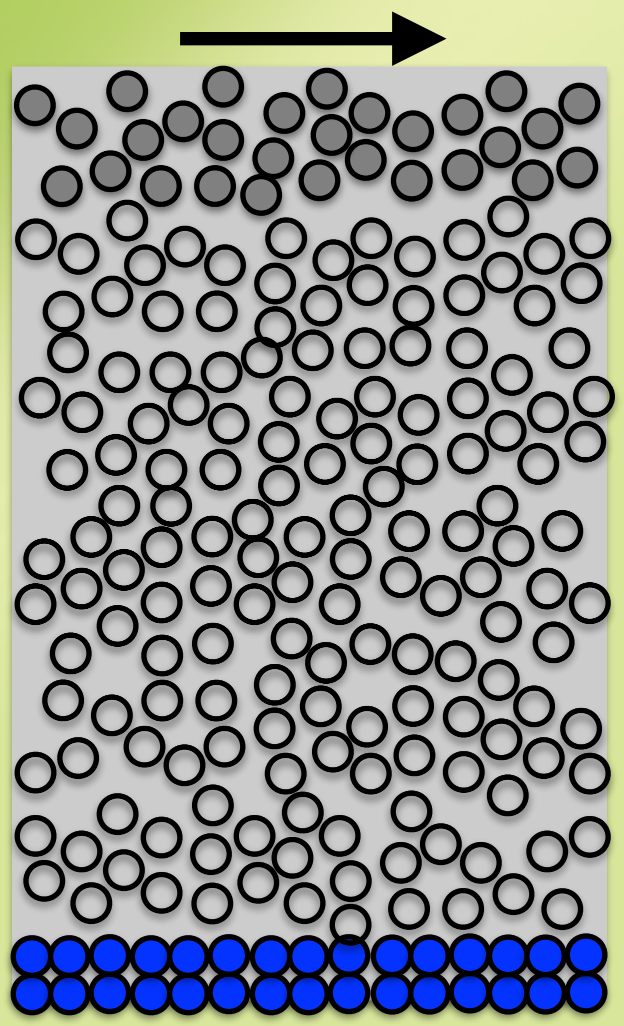
Chen and Doolen, Annu. Rev. Fluid Mech. 30, 329 (1998)

Lattice Boltzmann method

Force on atoms:

$$\vec{F}_k = -\nabla_k U\left(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N\right) = -\nabla_k \sum_{j>i=1}^{N} \phi_{ij}\left(r_{ij}\right)$$

$$\phi_{ij}\left(r_{ij}\right) = 4\varepsilon_{ij}\left(\left(\sigma_{ij}/r_{ij}\right)^{12} - \left(\sigma_{ij}/r_{ij}\right)^{6}\right)$$



Solve Newton's equations:

$$m_k \frac{\partial^2 \vec{r}_k}{\partial t^2} = \vec{F}_k\left(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N\right)$$

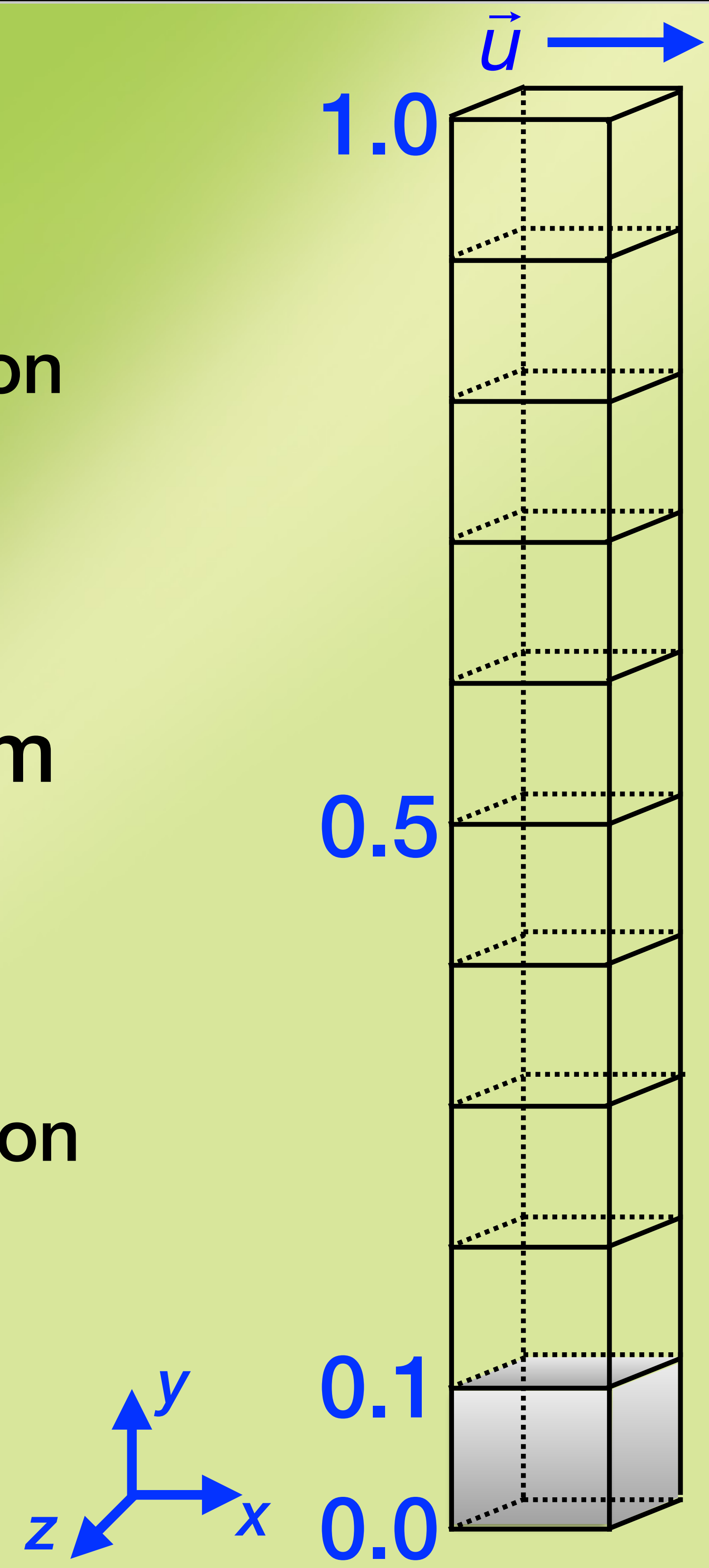
$$\vec{r}_k\left(t + \Delta t\right) = \vec{r}_k\left(t\right) + f\left(\vec{F}_k\left(t\right), \Delta t\right)$$

Discrete time steps:

$\Delta t \sim 10^{-15}$ - 10^{-14} seconds

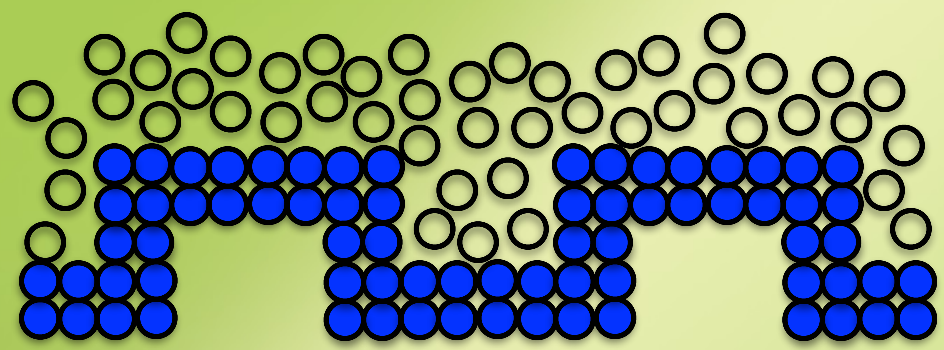
e.g., LeSar, Introduction to Computational Materials Science (Cambridge, 2013)

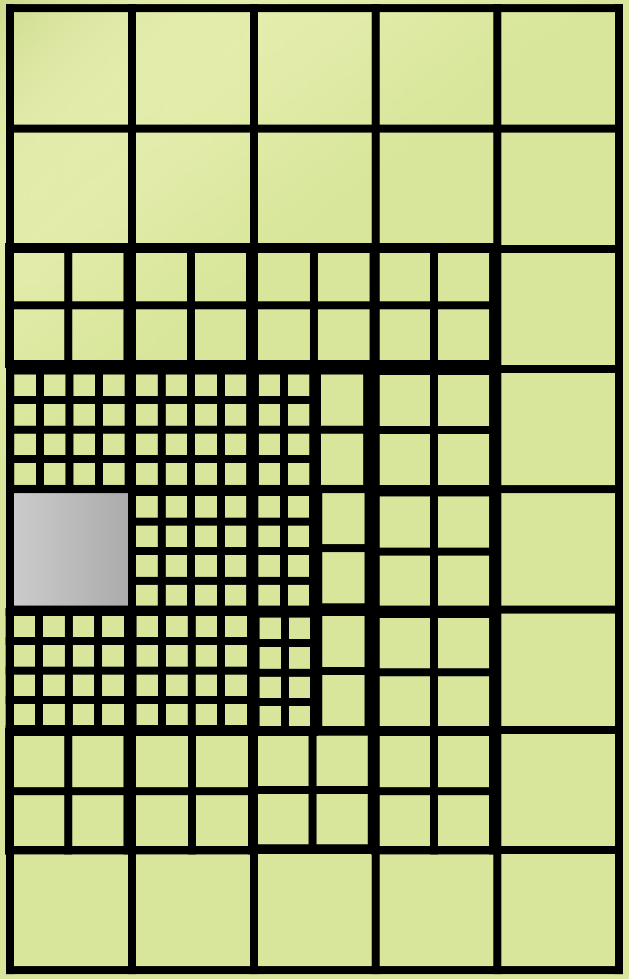
- Lattice Boltzmann solved on the 3D grid (one column shown)
  - upper velocity set as a boundary condition (u = 1)
  - LB yields the velocity at top of MD cell
- Molecular dynamics solved in bottom grid volume
  - determines the velocity at fluid/solid interface
  - that velocity sets lower boundary condition for LB
- Iterate until converged solution



Boundary between LB/MD

- Varying strength of solid/fluid interaction (potential parameters)
- Effect of the roughness of the surface on the fluid flow
- Extend the LB/MD method to larger scales using standard multigrid methods.

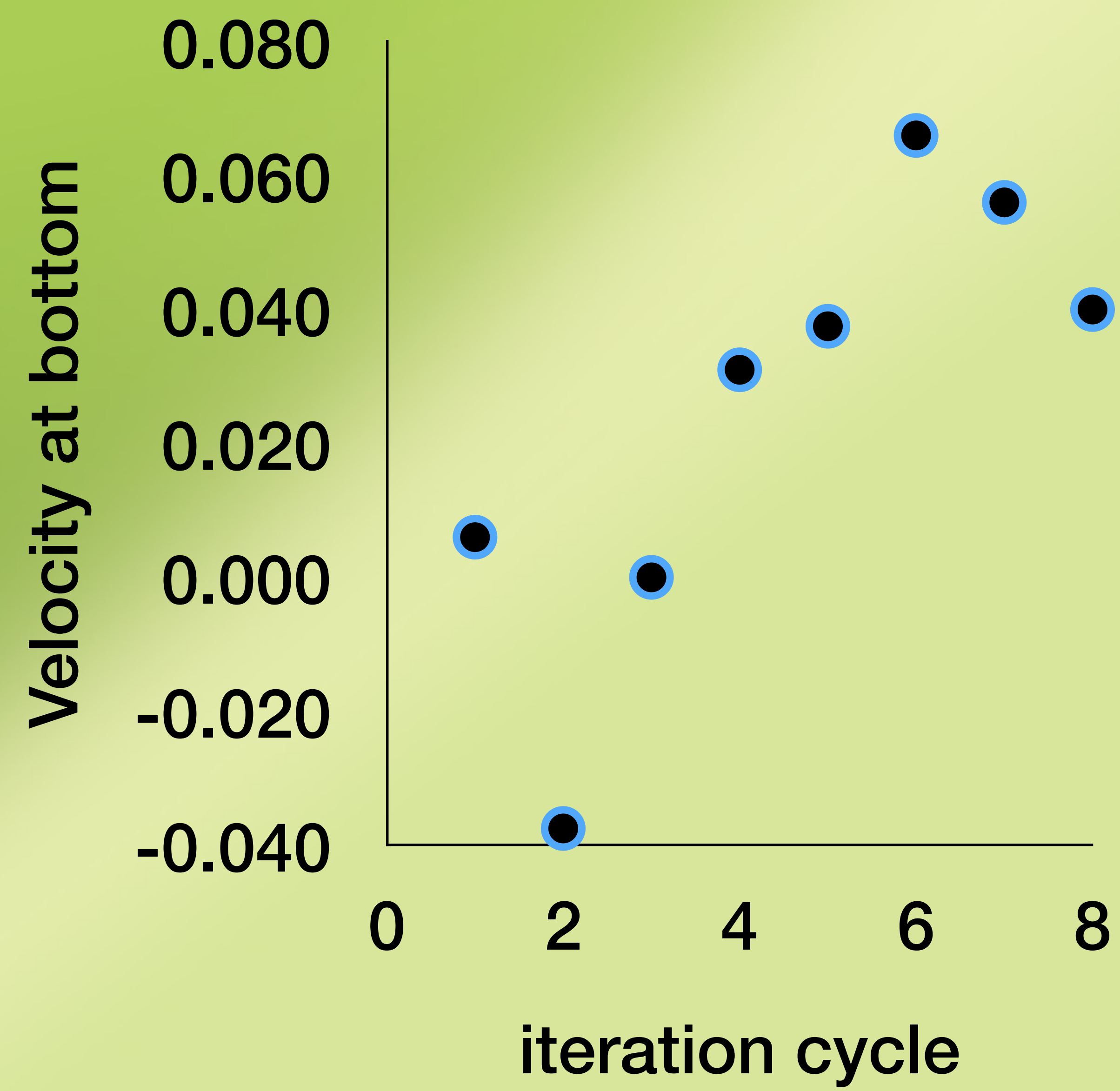




e.g., Asproulis et al., Advances Engin. Software 46, 85–92 (2012)

- Our current focus is on understanding the boundary between the methods
  - convergence
  - stability

- Examining different methods of coupling
  - gradient



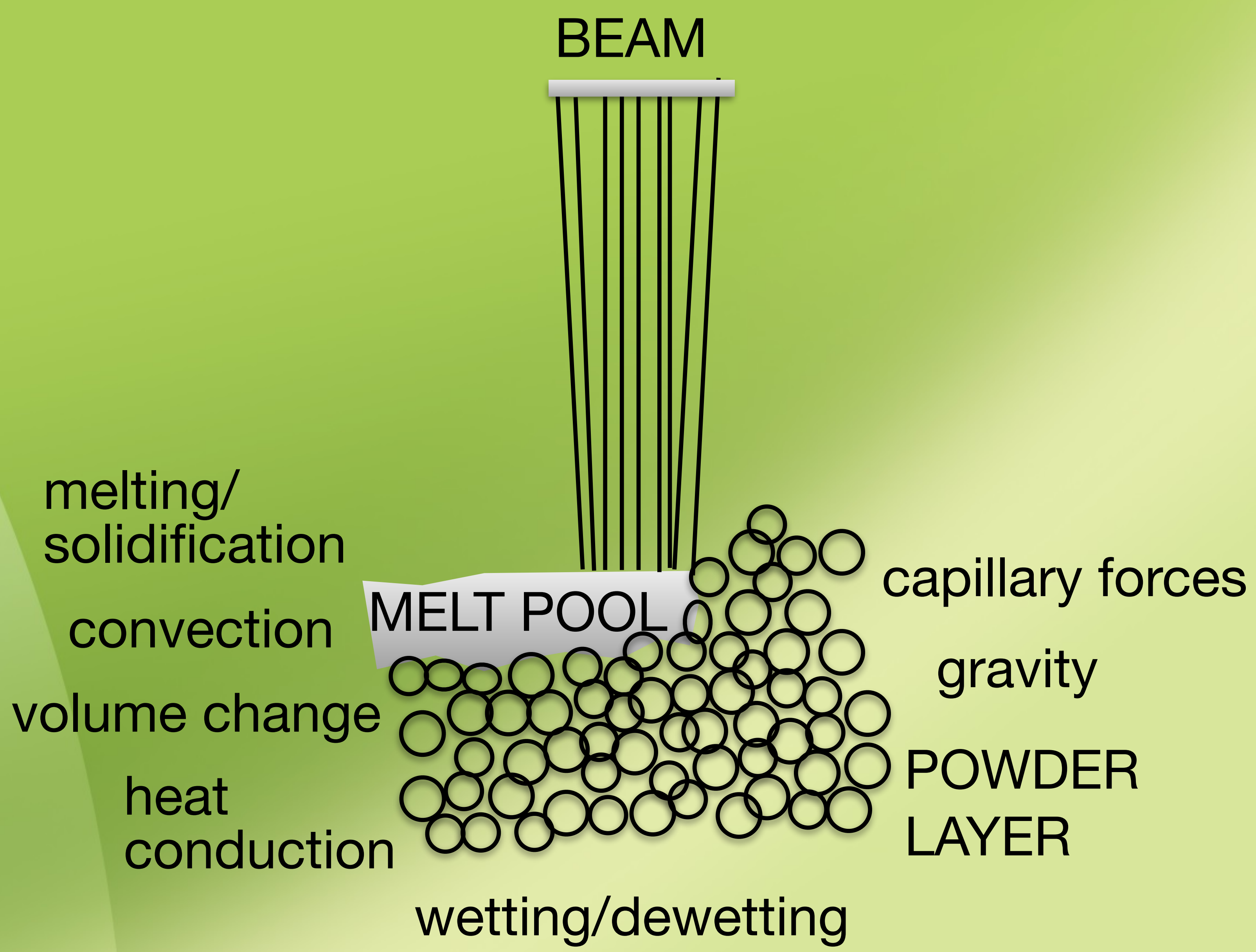
fluid-solid interaction 0.75 of fluid-fluid interactions

Convergence

- create independent models
- develop language for model-model communication
  - compatibility of information
  - boundaries
  - convergence
  - stability
- "snap" models together
  - substitute different models

mediation

Path forward



Körner et al, J. Mater. Processing Tech. 211, 978–987 (2011)

Additive manufacturing design tool

- “Accurate” simulation and modeling of real systems
- Interactive decision tools
- Realtime communication and decision making
- Easily understood graphical interface

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