Collaboration for Multiphase Flow Research: Computational Physics and Application

Ray Cocco
Particulate Solid Research, Inc.

Christine Hyrena
University of Colorado at Boulder

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Vision

- Ensure that by 2015 multiphase science based computer simulations play a significant role in the design, operation and troubleshooting of multiphase flow devices in fossil fuel processing plants

Objective and Deliverables

- Discuss outstanding research problems in <u>implementing</u> computational multiphase flow applicable to fossil fuel processing
- Develop an emerging technology roadmap for <u>implementing</u> computational multiphase flow
  - What do we have today?
  - What will we need to have?
- Develop the plans for a collaboratory based roadmap
  - How are we going to get there as a team?

Discussion Topics

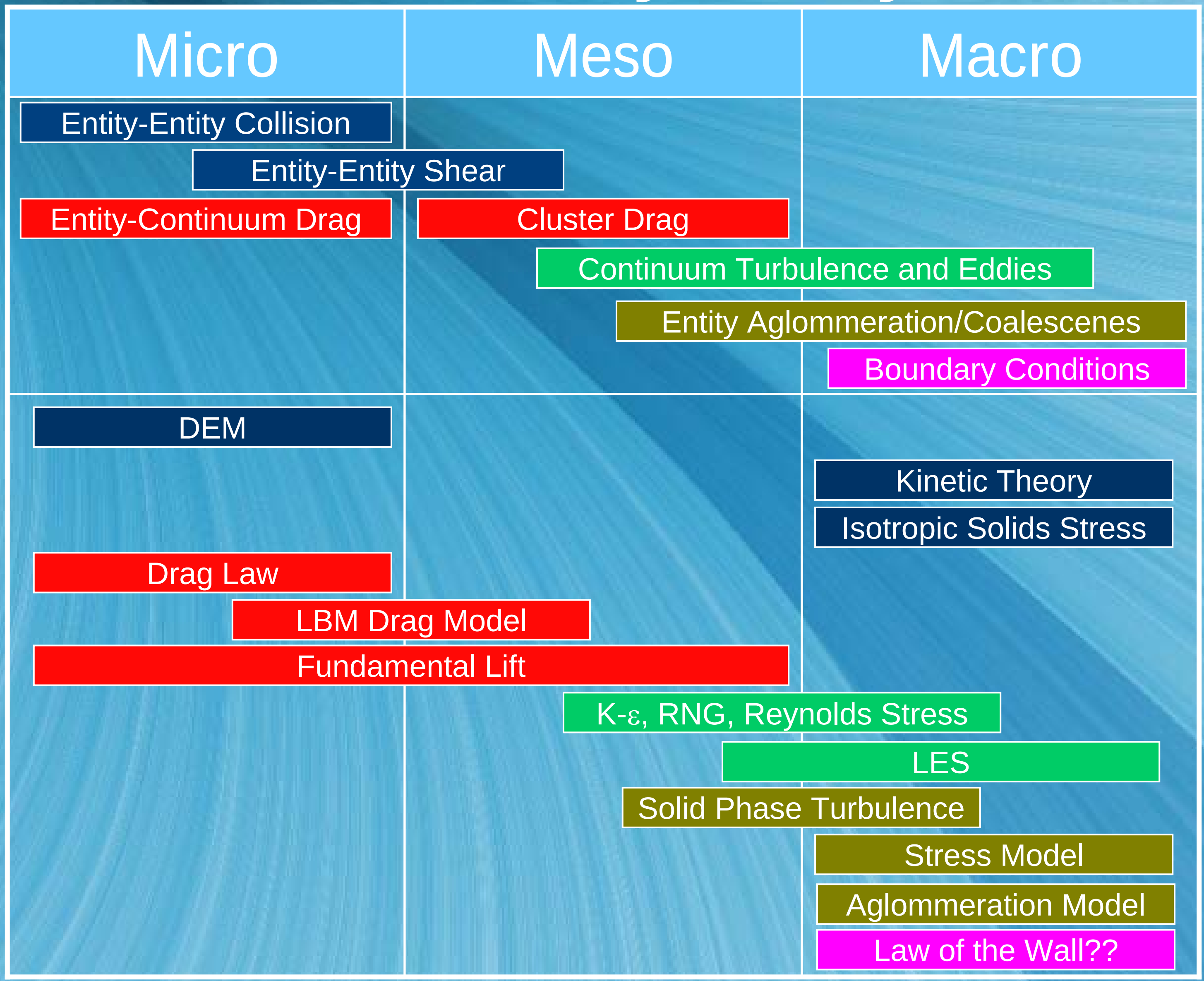
- How to best exploit the enormous amount of data generated by simulations?
- Research Topics
  - Numerical techniques
    - Eulerian-Eulerian, Lagrangian-Eulerian, DEM, LBM, VOF, MP-PIC, Drift Flux, etc
  - Computational speed
    - Model limitations
    - Equipment limitations
  - Verification and Validation
- How to apply what we know in industry?
  - Identifying relevant problems
  - Outreach activities

What to do with the simulation data?

- Visualization
  - Is it just a good show?
- Process design integration
  - Aspen/CAPE
    - Using “empirical” models via simulation results
    - Using simulations to populate a manifold or predefined matrix
    - Direct integration with model
  - Statistical model
    - Parametric study
    - Design charts

Where are we now and where do we want to go?

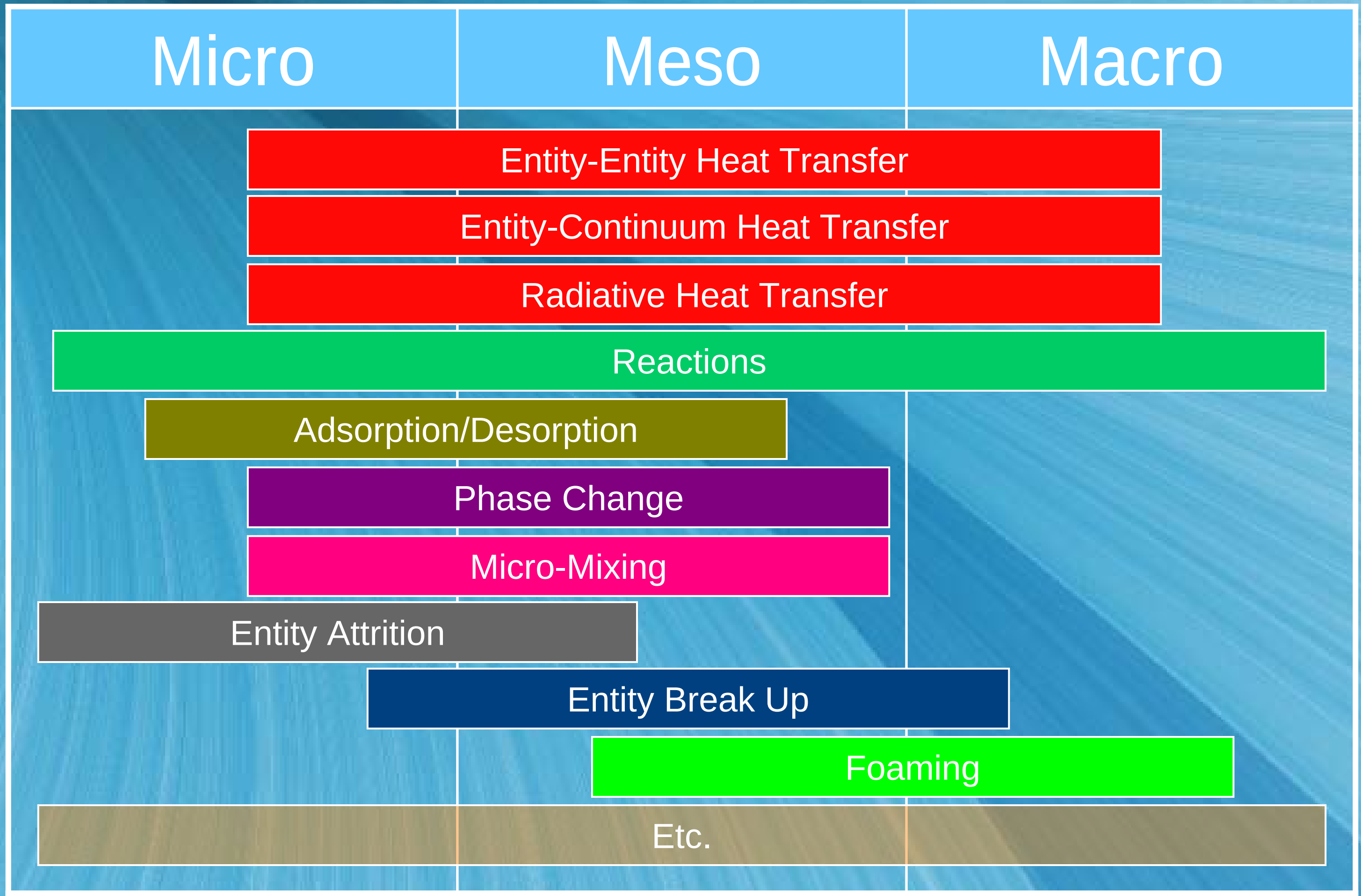
How to do the hydrodynamics?



This is by no means all inclusive

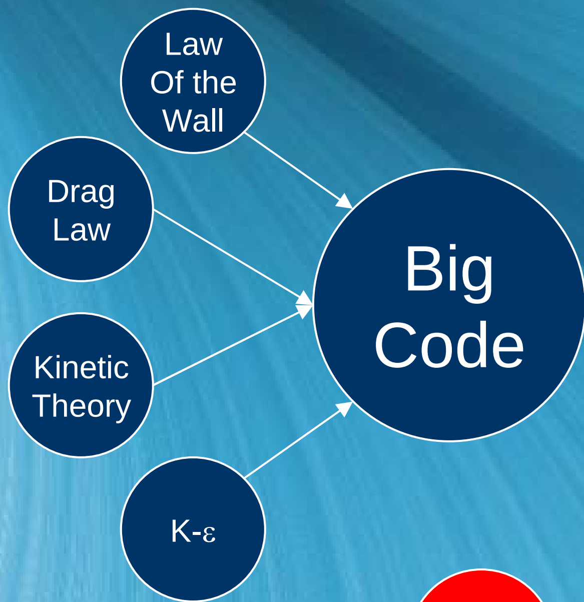
Entity is the lesser phase such as a particle or bubble

And what about?



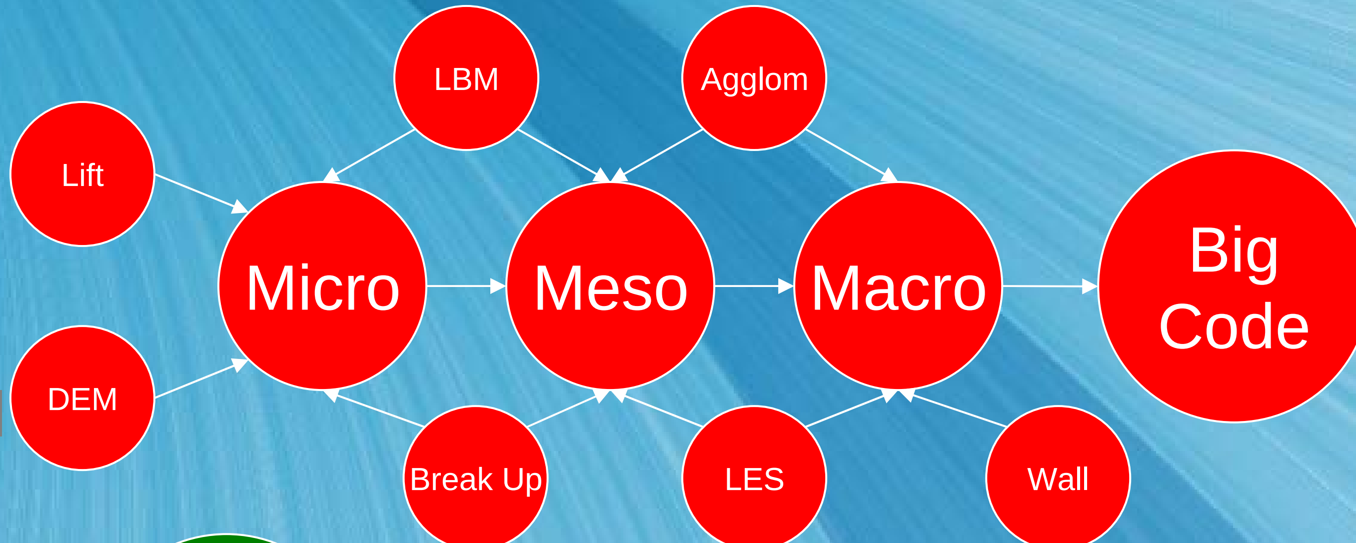
- Where do we start?
- Where to we stop?

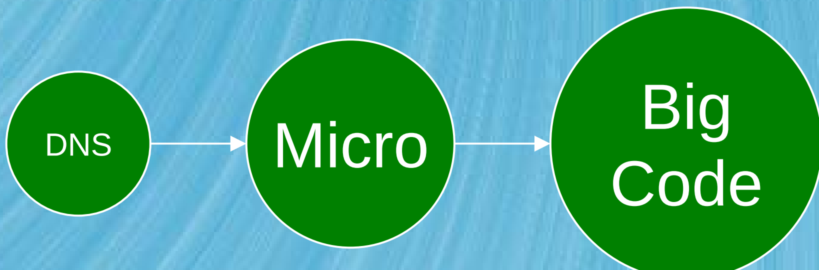
Can we do this with one code?



Generalized constitutive equations bridge the gap between scales (today's models)

System specific constitutive equations are generated internal for each scale

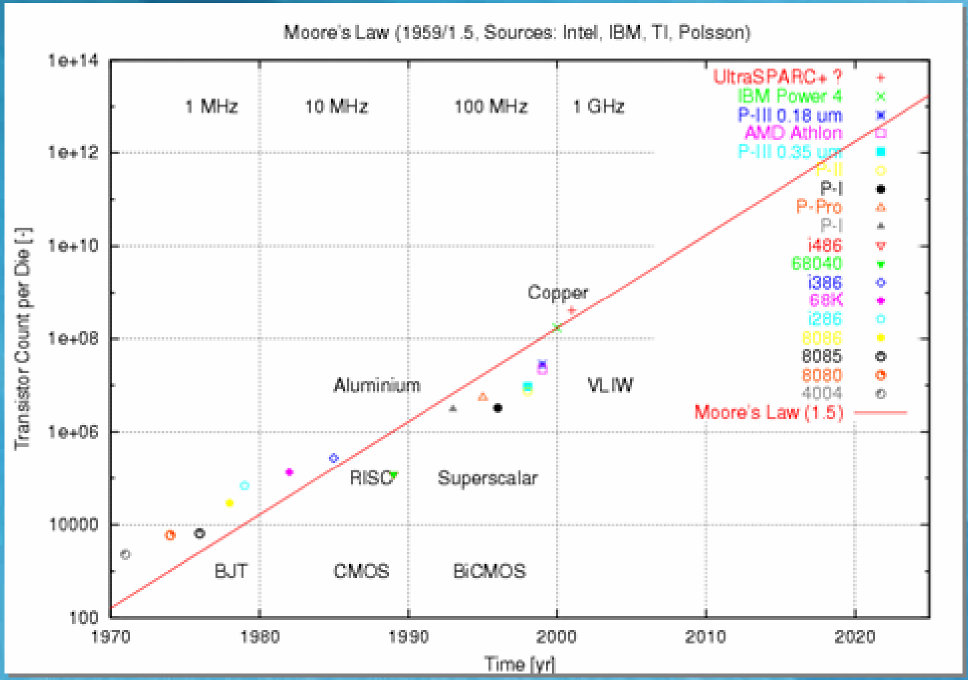




Pure fundamental code

By 2015?

What type of computer architecture are we shooting for?



- Do we really need to design for parallelized processors?
  - Blocking
- Will CPU outpace the requirements of accurate models (I.e., reactions, etc.)?

How do we verify and validate the model(s)?

- “No one believes the models except the modelers, everyone believes the experiment except the experimentalist” - A. Einstein
- Is experimental data good enough?
  - Large scale
    - Accuracy, reproducibility, electrostatics, leaks, etc.
  - Small scale
    - Scale up effects, segregation, etc.
- Are we doing the right experiments or are we just using what is out there?
  - I.e., drag law

Modelers need to direct some experiments

How do we verify and validate the model(s)?

- Your model is not validated just because your similar one or two cases
  - But how much data do we need and when are we done?
- Validation needs to be done on multiple scales otherwise is really is not a scale up tool
  - Where do we get large scale data?
    - Industrial reactors are not equipped to provide the needed data (except reaction productivity)
- Must do parametric studies first
  - Does the sensitivity to input parameters make sense?
    - Coefficient of restitution is just one example
  - Need to understand the controlling sources of error and uncertainty
- How do we handle resolution?
  - CPU vs accuracy
- Do we need tools for error, cpu requirements, resolution?
  - Idiot proofing the model

How to apply the model(s)?

- Incremental research
  - Start small and work your way up
- “Buy in”
  - Let industry help with finding the right problems as you work your way up
- Have a realistic economical model
  - Cost vs. gains
  - Include resource loads
- Have an outreach program
  - Internships for students with industry and national labs
  - Active sponsors with academia

Summary

- Lots of questions
  - How do we manage data mining?
    - Code integration into process tools (CAPE)
  - What type of model structure (empirical constitutive vs pure fundamental) will give us the accuracy at low CPU costs?
  - What type of cpu architecture should we be shooting for?
  - How far should our models go (reaction, attrition, micromixing, etc.)?
  - How do we validate and when do we stop?
  - How do we implement a validated model?
- A good model is one that makes the right assumptions of what NOT to include