# Applying Aerospace Knowledge to Unconventional Wells

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# **Rarefied Gas ≈ Nano-scale Pores**

# How we can use the HYBRID CONTINUUM-DSMC FRAMEWORK for unconventional wells?



## **Rarefied Gas ~> Unconventional Wells**

Knuder	so Num	hor Kn-	$\lambda_{n} = \frac{\lambda}{\lambda}$ Mean Free Path of Fluid Molecules					
Rituuse	$IDer. M^{n} = I$	$\Lambda$ Macroscopic-Average Pore-Diameter						
C	No-Slip onditions	Slip Condition	s					
Continuum Flow		Slip Flow		Transitional Flow		Free-I F	Free-Molecular Flow	
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0 <b>€</b> Kn	1	0 <sup>-3</sup> 10 <sup>-2</sup>	1	0 <sup>-1</sup> 1	00	<b> </b> 10 <sup>1</sup>	Kn <b>→</b> ∞	
Non-Darcy Flow	Darcy Flow	Non F	-Da lov	rcy v				
Macro-so		Nano-scale pores						
Fast-Evolvin	es	Slow-Evolving Processes						
Fluctuation	le	Fluctuations significant						
Averaging	ing F	Pore-scale characterization						
Domain-scale modeling		ng	Por		e-scale modeling			
Bulk properties			Inti		insic properties			
Continuum Flow		DSMC	DSMC		Rarefied Flow			
Navier Stokes		Navier Stokes		DSMC				

- Can use either DSMC or N-S (with slip effects) between  $10^{-3} 10^{-1}$
- Continuum model requires adequate slip boundary treatment in this region
- Cost is cheaper the higher the Knudsen number at which Continuum/DSMC interface occurs



## **DSMC: Direct Simulation Monte Carlo**

- Particle-based technique for simulating rarefied fluid flows
  - Knudsen number~0.1 or greater => rarefied flow
  - Low density fluids => large spacing between molecules (Aerospace)
  - Small pore size => large spacing between molecules (O&G)
- Simulation molecules ~ large number of real molecules => probabilistic simulation to solve Boltzmann equation.
- Intermolecular collisions and molecule-surface collisions calculated using probabilistic models
- Fundamental assumption:
  - Molecular movement and collision phases can be decoupled over time periods that are smaller than the mean collision time



# **Modeling Approaches**

#### For high Kn, continuum models (N-S /Darcy) are not accurate

- Slip effects become important and flow does not equilibrate thermodynamically
- Continuum code over-predicts near wall features such as skin friction and heat transfer
- For low Kn, fully rarefied (DSMC) computations too expensive
- CRAFT Tech utilizes hybrid approach to cover all Kn
  - Continuum model within continuum regions (typically Navier-Stokes) with possible enhancements to extend range to more rarefied regimes
  - Rarefied model within rarefied regions (typically Direct Simulation Monte-Carlo)
  - Coupling occurs across interface surface or region
  - Mitigates numerical inefficiencies
  - Modeling of important physical phenomena must be consistent across interface



Coupling Interface High Altitude Flow



#### Application to Nano-Porous Unconventional Reservoirs

- Flow within pores are in noncontinuum regime because geometric length scale is small
- For rarefied flow bulk, continuum transport properties (diffusion, viscosity, etc.) are no longer valid, requiring rarefied physical models
- Variation of length scale through extraction region also means there is mixture of continuum and rarefied regions
- Successful modeling of system requires hybrid analysis





## **Unsteady Interface Methods**





## **CRAFT Tech Hybrid Paradigm**

- Apply most accurate physical models in each region
  - Continuum Navier-Stokes (CRAFT CFD® / CRUNCH CFD®)
    - Turbulence modeling
    - Finite rate chemistry
    - Two-phase flows
  - Rarefied (Nanoscale) Direct Simulation Monte Carlo (DSMC) (HAMMRS)
    - Non-local thermodynamic equilibrium
    - Free-molecular flows
- Identify interface regions in generic fashion using Knudsen number based criteria
- Numerical efficiency and physical accuracy improved by optimizing the location of the interface region and advanced methods for exchanging information at the interface
  - Production level continuum-rarefied steady-state interfacing for even complex geometries and surfaces including two-phase flows through Automatic Efficient Generalized Interface Surface (AEGIS) Toolkit



#### Apollo Capsule Reentry Interface Surface Generation Interpolation



Mach Number (Clipped Below Sonic)



Mach Number (Clipped Below Sonic)

**Velocity Vectors** 



# Generalized EOS (Continuum Flows)

# Experience with multi-phase, multicomponent fluids



### **Thermo-Chemistry (Fluid Properties)**

- Generalized EOS models for mixtures of liquids and gases
- Compressible liquid EOS models
- Ideal gas EOS:
  - Extensive database based on 7-coefficient NASA polynomials
- Real fluid EOS based on SRK (Soave, Redlich and Kwong):
  - Supported species: hydrogen, nitrogen, oxygen, methane, ethanol and ethane
  - Additional species can be added to EOS framework

$$P = \frac{RT}{V-b} - \frac{a}{V^2 + ubV + wb^2}$$

where

- R = universal gas constant
- V = molar volume
- u and w = model constants depending on PR or SRK
- a and b = constants for a given substance which maybe a mixture in which case they are dependent on mixture composition



### **Combustion Modeling – How It Works!**

A framework for simulating an impingement atomization/combustion sequence



Combustion

#### Schematic of the Injector/Combustion Sequence



#### **Combustion Modeling – How It Works!**

**Red** =  $CH_4$  sheet Orange =  $CH_4$  droplets Yellow =  $CH_4$  vapor Blue = LOX sheet Metallic = LOX droplets Aqua =  $O_2$  vapor





## Summary

- DSMC and hybrid DSMC/Continuum technology can potentially be applied to modeling nano-porous unconventional reservoirs with additional technology development
- Characterize pores of different scales with DSMC or hybrid DSMC/Continuum procedures
- Integration into fast running system tools can potentially be achieved by using DSMC calculations to provide calibration of permeability as a function of porosity and pore size
- Framework for generalized EOS in place and easily modified for O&G fluids
  - Extensive experience with multi-phase, multi-component fluids

