Direct Numerical Simulation of CO2 Diffusion in Reconstructed Solid Sorbent Particles

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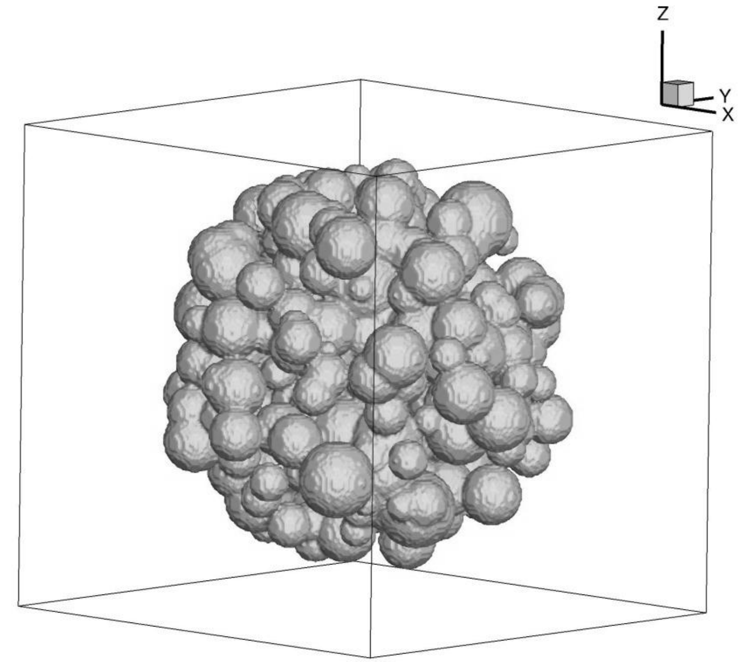
Introduction

- **Post-combustion carbon capture methodologies**
  - Solvent based processes
  - Solid sorbents
    - Metal oxides
    - Amines on porous support base
    - …
  - Membranes
  - …

Introduction

- **Complex porous microstructures**
- **Multi-scale nature**
  - Macro – particles sized a few 100 microns
  - Meso – channels sized 5-50 nm
- **A variety of physical phenomena involved**
  - Fluid flow
  - Heat and mass transfer
  - Surface kinetics
  - …



A porous spherical particle created using stochastic reconstruction with a porosity of 0.40

Introduction

- **Numerical tools**
  - Use of realistic porous microstructures
  - Capability to perform simulations through these complex geometries
- **Understanding the involved physical processes**
  - Importance of realistic geometries
  - Effects of porosity, microstructure characteristics etc.
  - Adsorption and desorption

Approach

Macro-scale modeling

- Recreate realistic porous particle geometries
- Heat and mass transfer simulations

Meso-scale modeling

- Adsorption/desorption model
- Knudsen diffusion

Carbon capture physics in solid sorbents

Approach

Macro-scale modeling

- Recreate realistic porous particle geometries
- Heat and mass transfer simulations

Porous reconstruction

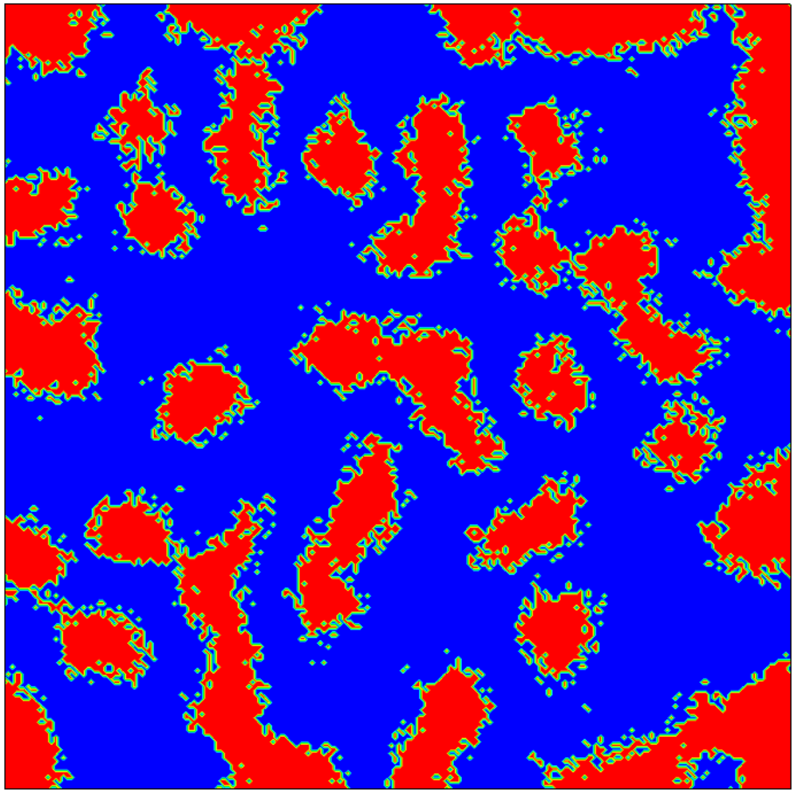
- Stochastic reconstruction
- Experimental imaging for input correlations

GenIDLEST + IBM framework

- Species diffusion
- Conjugate heat transfer
- Parallelization

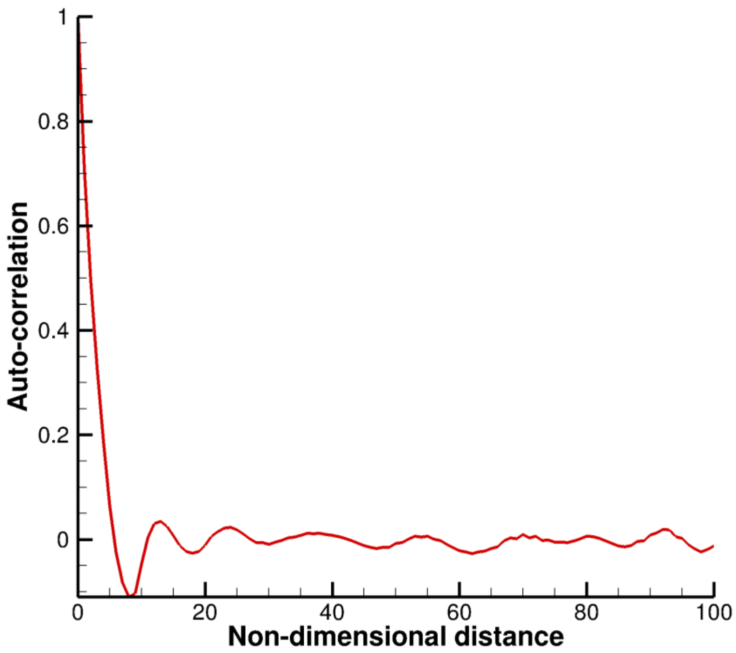
Stochastic reconstruction

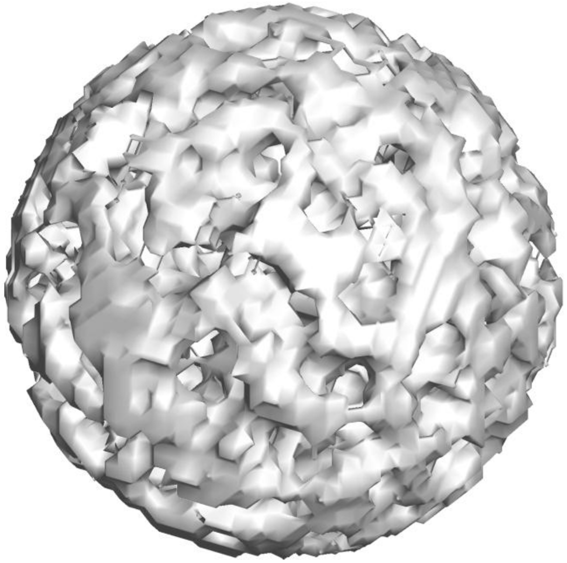
- **Use of a stochastic reconstruction method – simulated annealing**
- **Input – experimentally determined auto-correlation function (ACF)**
- **Initial – random field with desired porosity**
- **Final – porous structure with desired porosity and auto-correlation**



A 2D porous medium generated with a porosity of $\varepsilon = 0.55$

Stochastic reconstruction



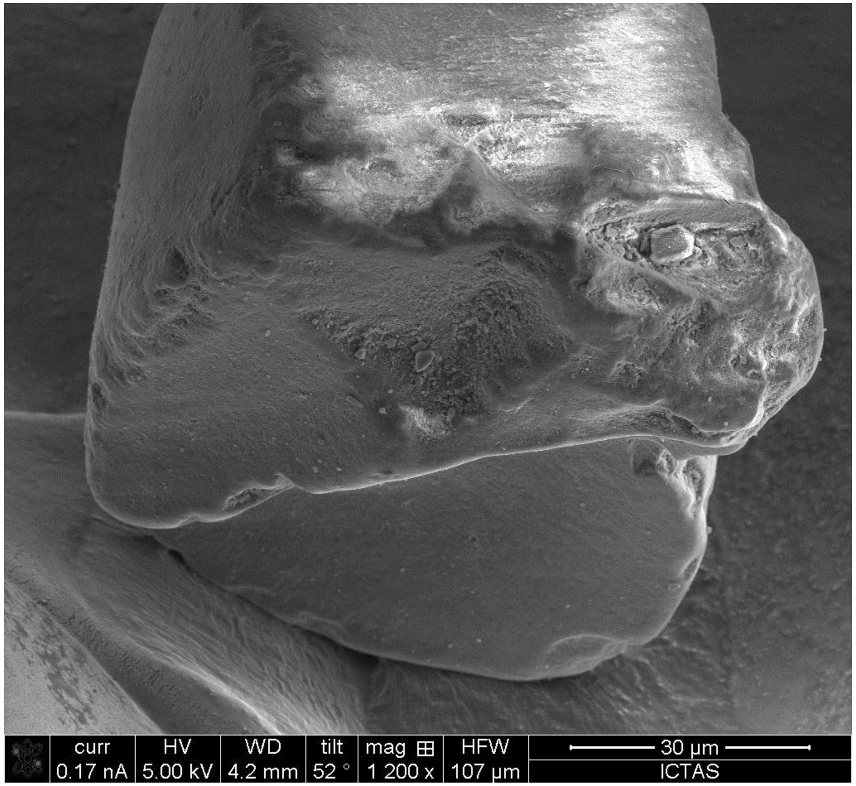


Input auto-correlation function created based on a recreated 2D image

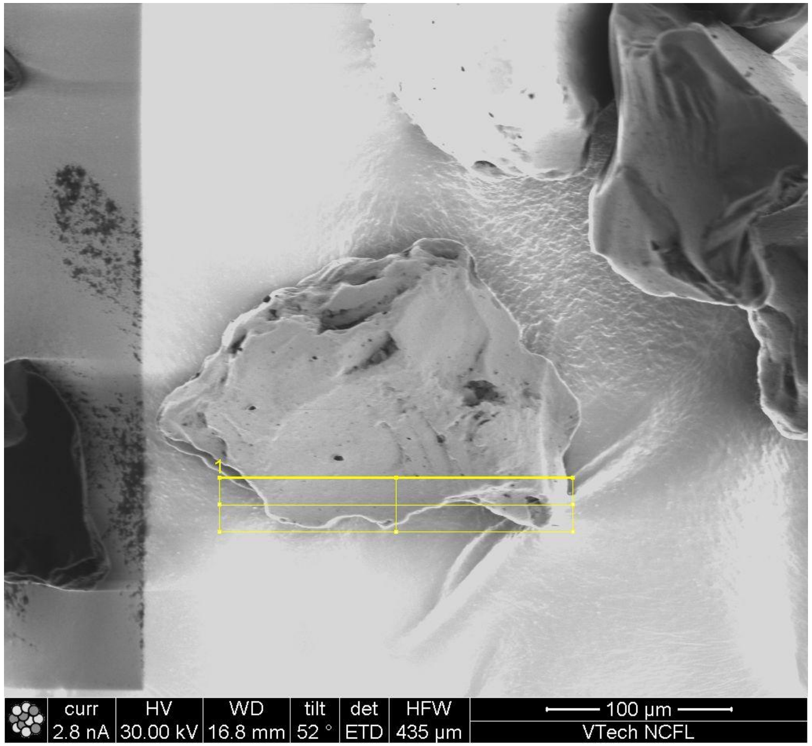
Stochastically reconstructed porous spherical particle with porosity of 0.55

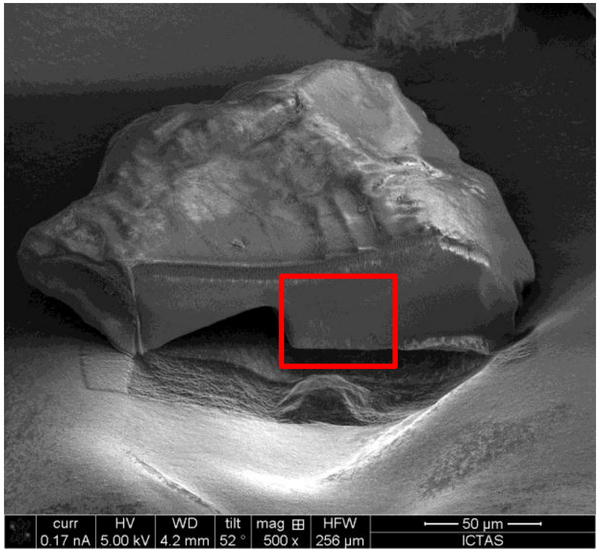
Experimental imaging

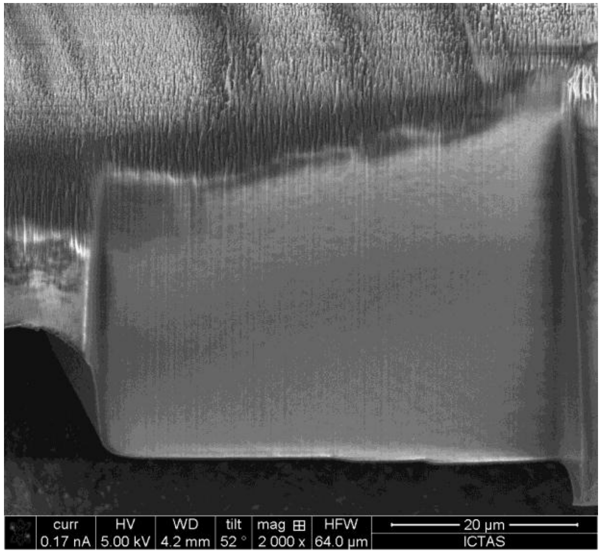
- **FIB-SEM imaging using FEI Helios 600 Nanolab at NCFL, Virginia Tech.**
- **Resolution**
  - 0.9 nm @ 15kV
  - 1.4 nm @ 1kV
- **Surface contour and internal microstructure characterization**



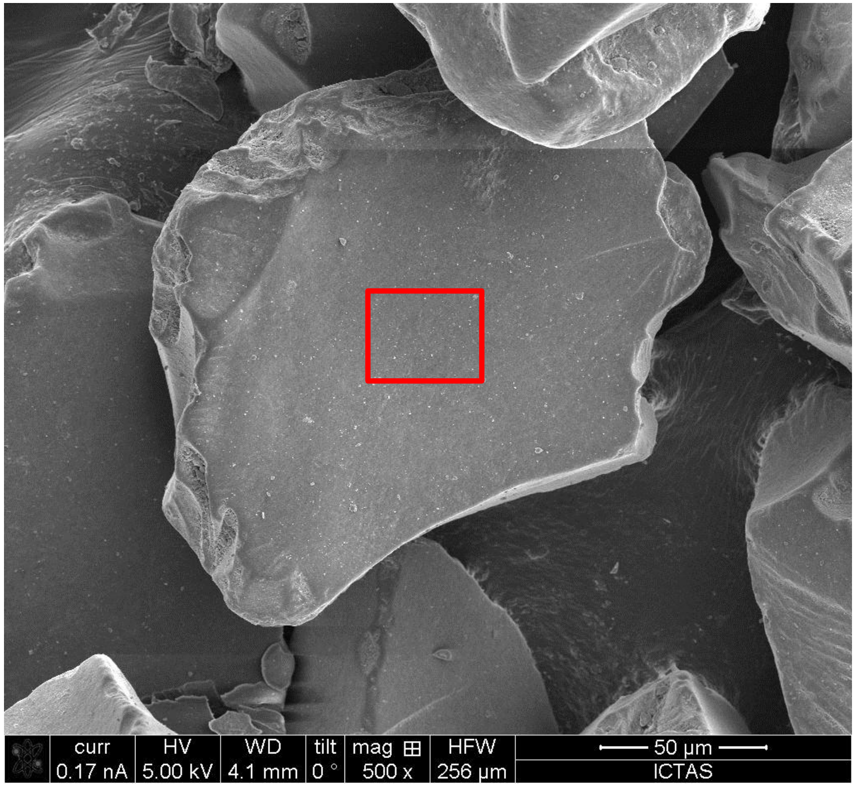
Experimental imaging – Sectional view

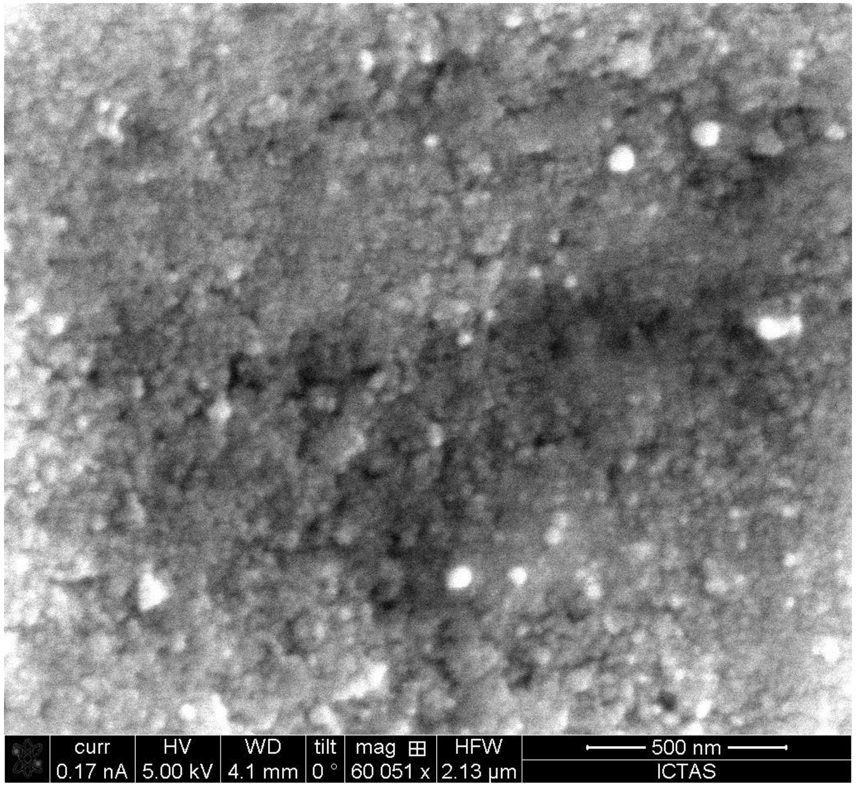






Experimental imaging – Surface contour





Approach

Macro-scale modeling

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Porous reconstruction

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GenIDLEST + IBM framework

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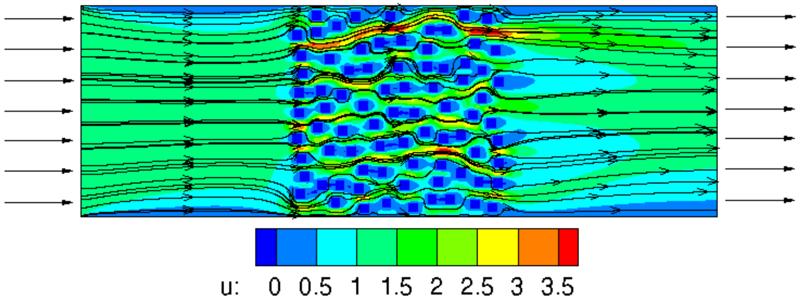
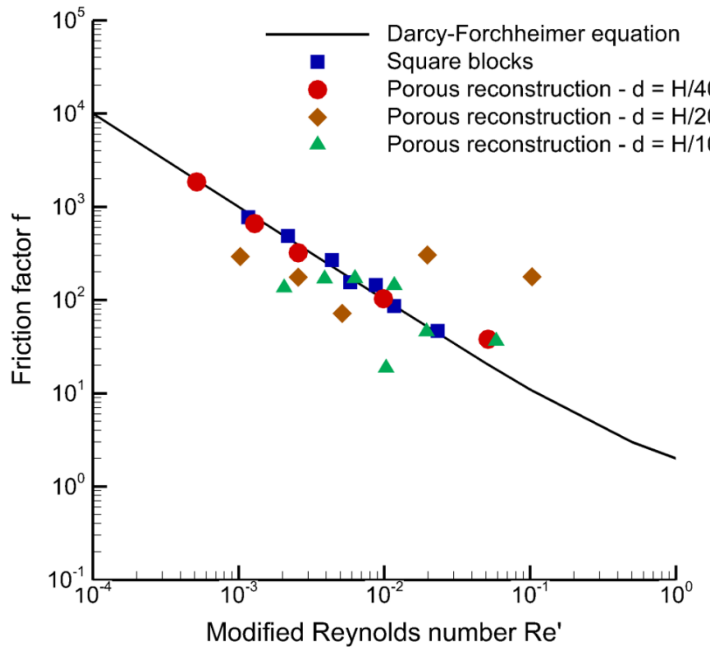
- Conjugate heat transfer
- Parallelization

2D Porous Channel Flow

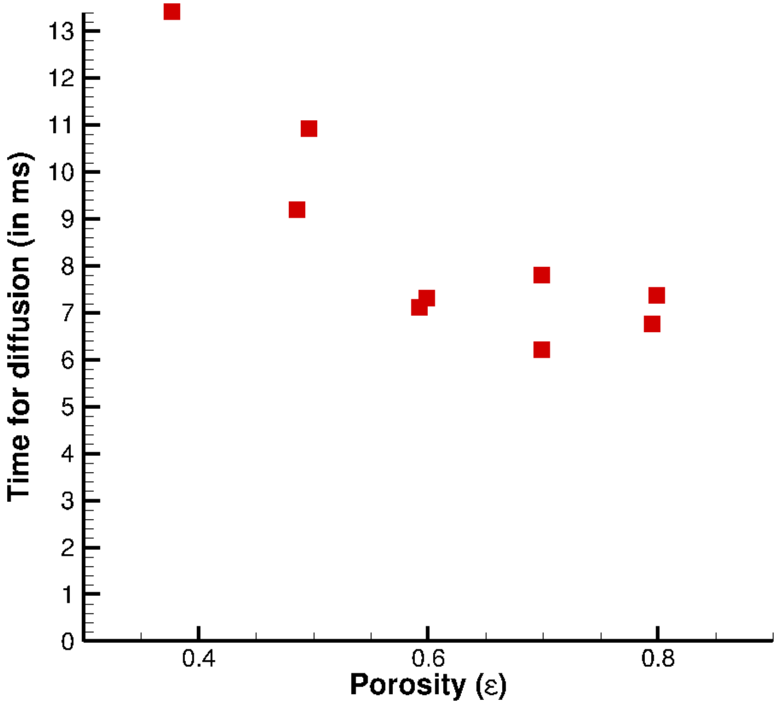
- **Flow through porous channels**
- **Friction factors for different flow Reynolds numbers**
  - Random arrangement of regular (square) blocks
  - Stochastic reconstruction
  - Analytical solution due to Darcy-Forchheimer equation





Species diffusion – 2D

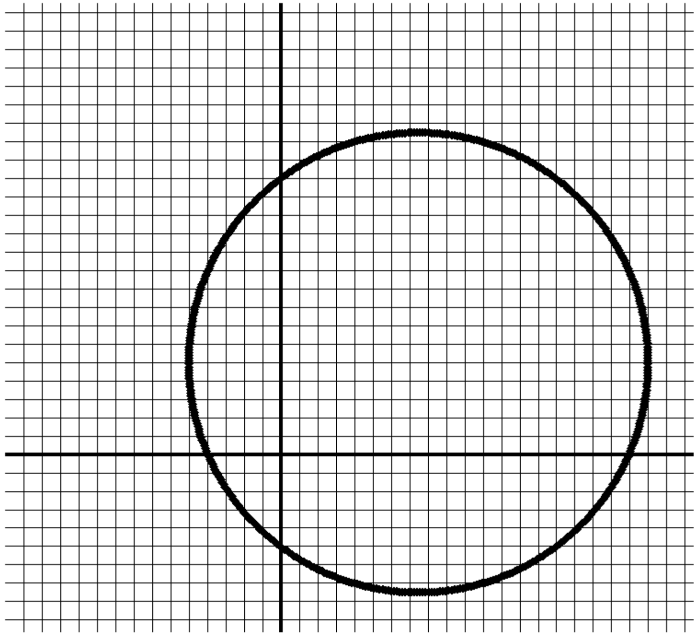
- **Porous particles (2D)**
  - 500 micron diameter particle
  - Ambience conditions – 15% CO_2
  - Initial conditions – 0% CO_2
  - Monitoring CO_2 concentration levels within the particle
  - Time for 95% CO_2 level saturation in the porous particle



Diffusion times observed for a 500 micron 2D porous particle with varying porosities

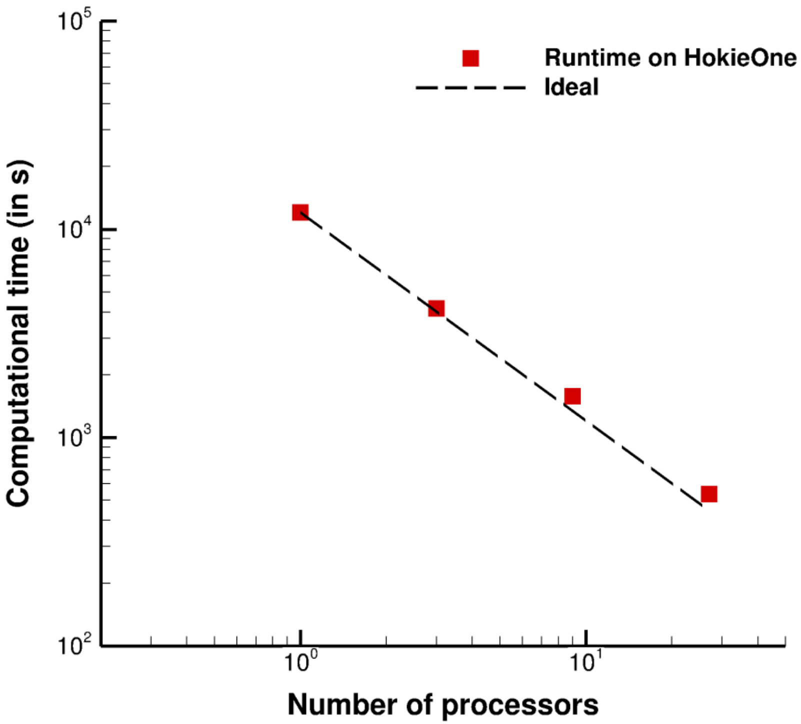
Parallelization

- **3D simulations – computationally very expensive**
  - 7.2 million cells for 3D porous particle case
  - 20+ days of computational time on 1 processor
- **Domain decomposed MPI parallelism – in line with GenIDLEST framework**



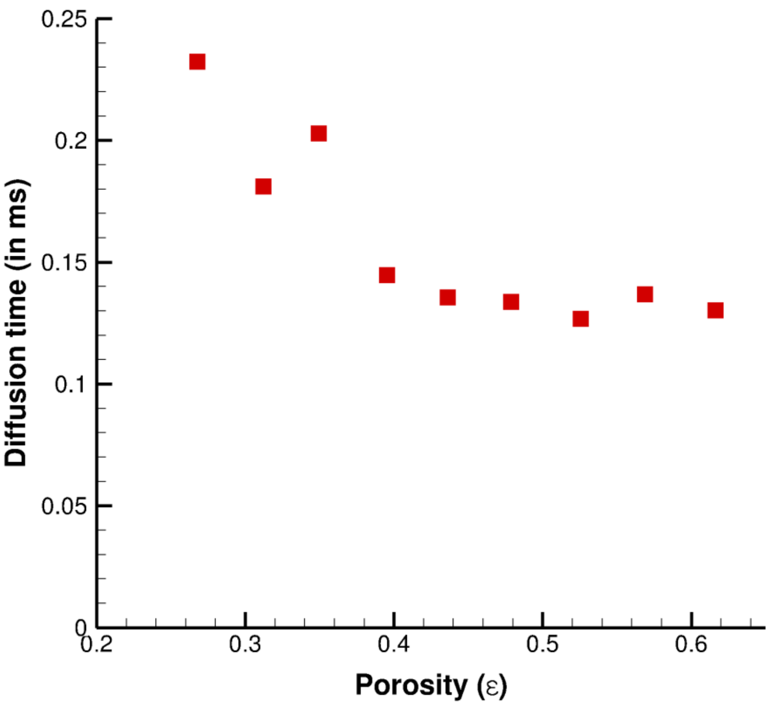
Parallelization

- **Strong scaling study**
  - Species transport problem through porous spherical particle
  - 7.2 million cells divided across a max. of 27 blocks
  - HokieOne
    - Shared-memory SGI UV system
    - 2.66Ghz Intel Xeon cores
    - 6 cores and ~30 GB memory per node
  - Computation time for 100 time-steps



Species diffusion – 3D

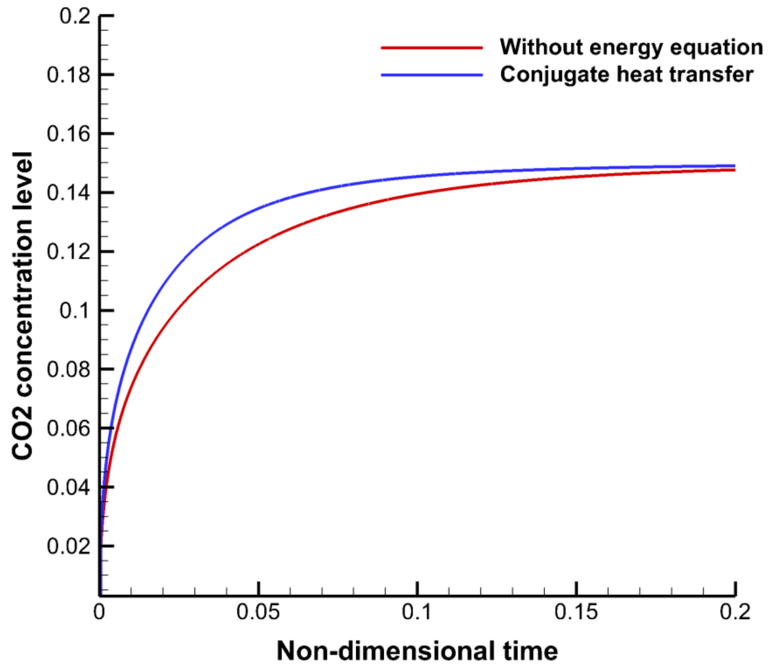
- **Porous spherical particles**
  - Same conditions as for 2D case
  - Porosity values of 0.20-0.60
  - 100 microns diameter



Diffusion times observed for a 100 micron spherical porous particle with varying porosities

Effect of Temperature Field

- **Inclusion of energy equation solution**
  - Constant temperature BC
  - **Conjugate heat transfer**
- **Conditions**
  - Particle temperature at 398K
  - Initial fluid temperature – 298K
- **Diffusion time reduction due to higher temperatures**



Summary

- **A numerical framework for macro-scale porous media**
  - Stochastic reconstruction of porous microstructures
  - Experimental imaging to obtain input correlations
  - Fluid flow, species transport and (conjugate) heat transfer simulations
  - Flows through porous channels, particles etc.
  - Parametric studies

Future work

- Alternate imaging techniques for digital reconstruction
- Models for surface adsorption/desorption and the related kinetics
- Modeling meso-scale effects and coupling with macro-scales
- Simulations to produce correlation maps to be used for large scale simulations

Acknowledgements

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Thank you!

Questions?