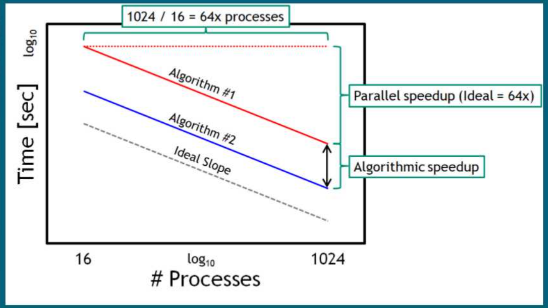
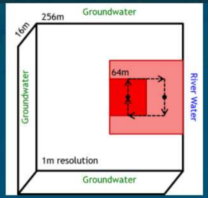
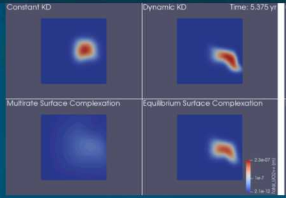
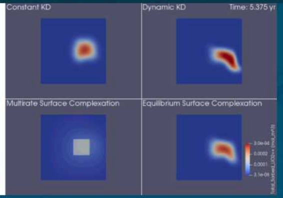
SAND2020-1056PE

Bounding Computation and Complexity for Reactive Transport on Supercomputers: A Perspective from Nuclear Waste Repository Performance Assessment









Sorption Model	Prescribed Uniform Flow		Heterogeneous Flow Field	
Constant K_D	Operator Split	Global Implicit	Operator Split	Global Implicit
Dynamic K_D	Operator Split	Global Implicit	Operator Split	Global Implicit
Equilibrium Surface Complexation	Operator Split	Global Implicit	Operator Split	Global Implicit
Kinetic Multirate Surface Complexation	Operator Split	Global Implicit	Operator Split	Global Implicit

PRESENTED BY

Glenn Hammond and Peter Lichtner*

International Workshop on: How to integrate geochemistry at affordable costs into reactive transport for large-scale systems

February 5-7, 2020

*OFM Research

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Overview

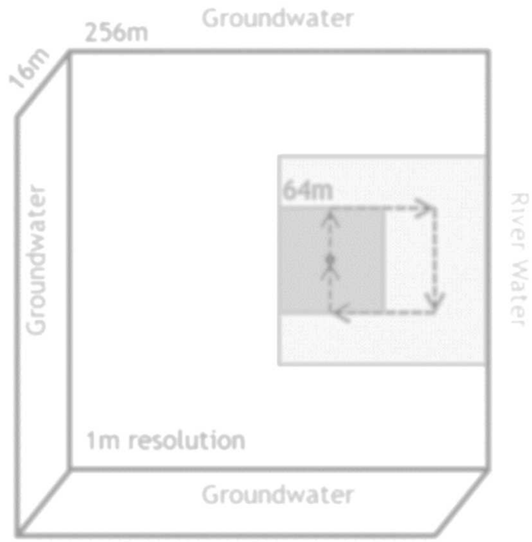
Motivation

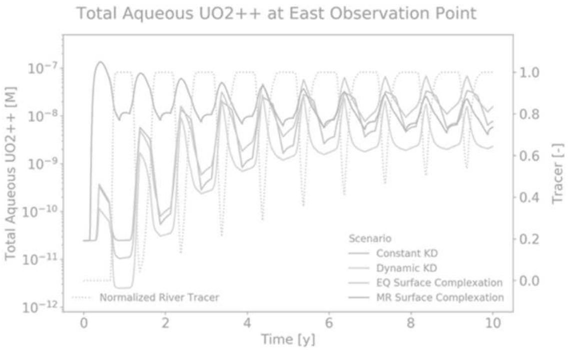
Hanford 300 Area test problem

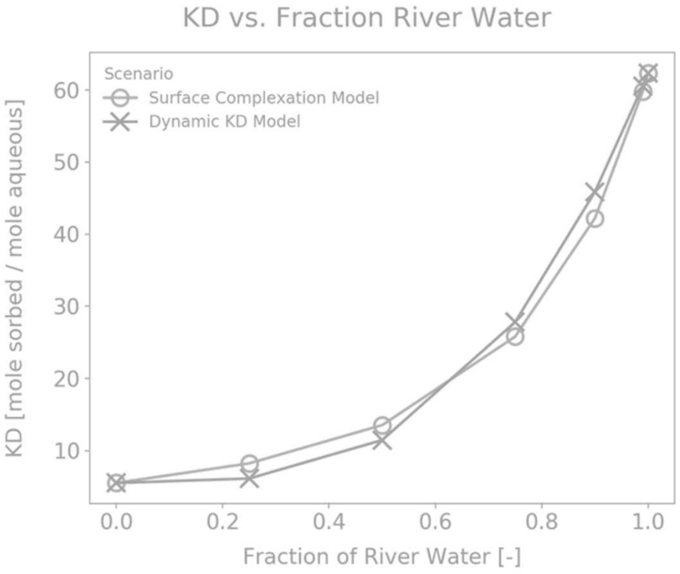
Prototype dynamic K_D model

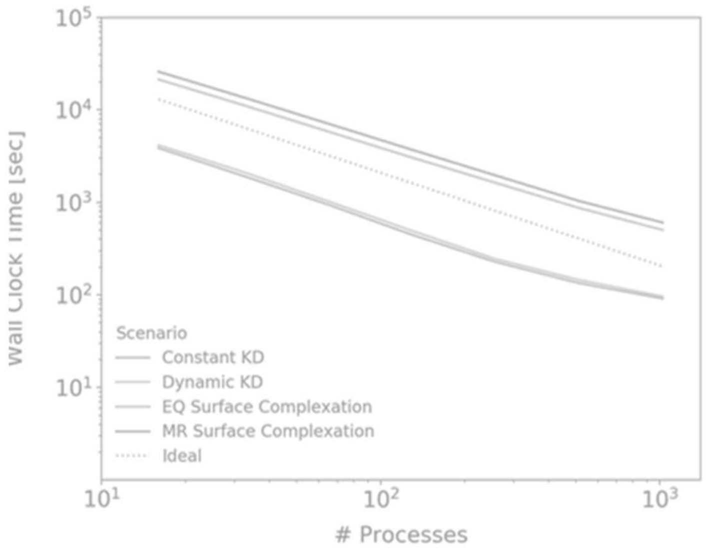
Parallel and algorithmic speedup results

Conclusion

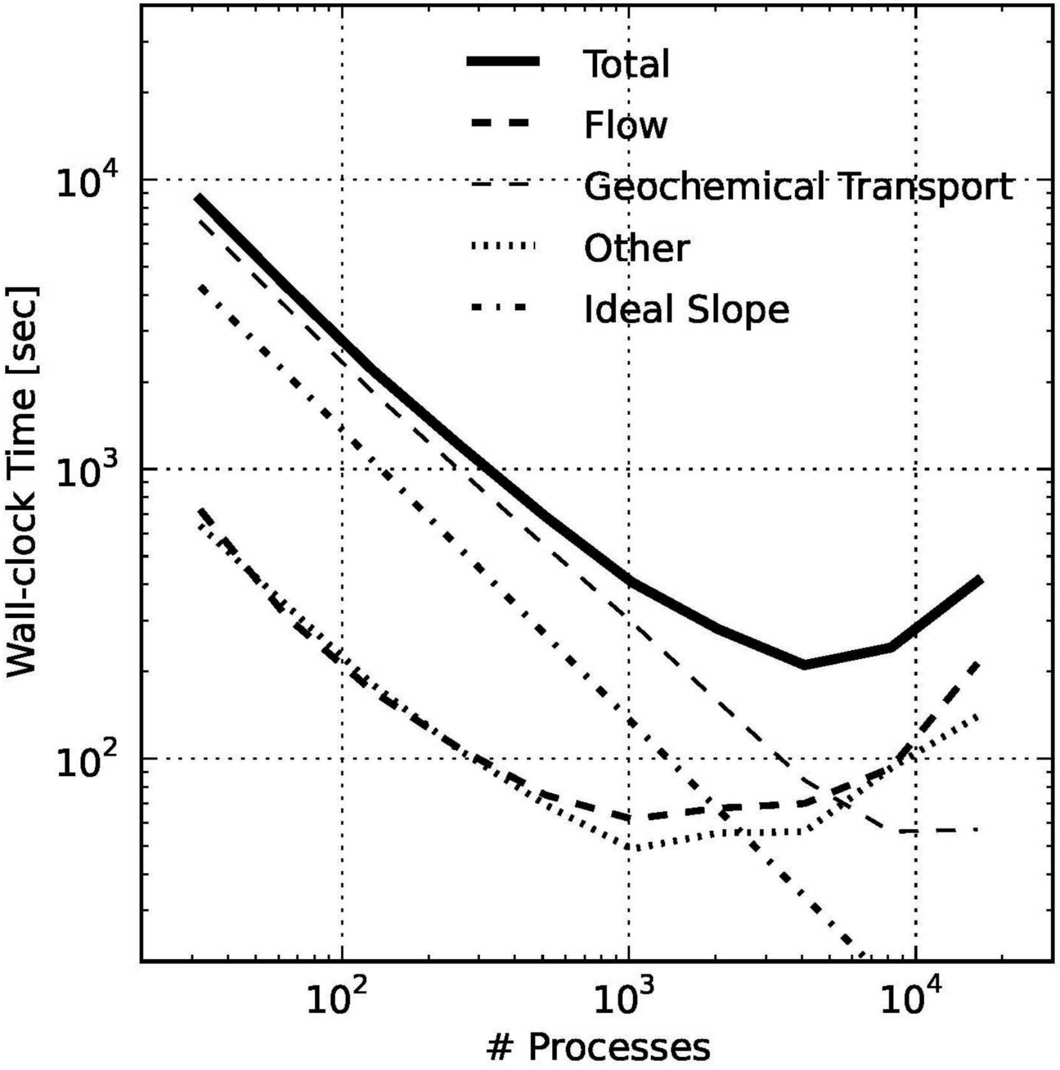








Motivation



Hammond, G.E., P.C. Lichtner and R.T. Mills (2014) Evaluating the Performance of Parallel Subsurface Simulators: An Illustrative Example with PFLOTRAN, Water Resources Research, 50, doi:10.1002/2012WR013483.

Questions

For a representative reactive transport (surface complexation) problem:

- What is the maximum speedup obtainable through parallel processing?
- What is the maximum speedup obtainable through simplification of chemistry?

PFLOTRAN

Petascale reactive multiphase flow and transport code

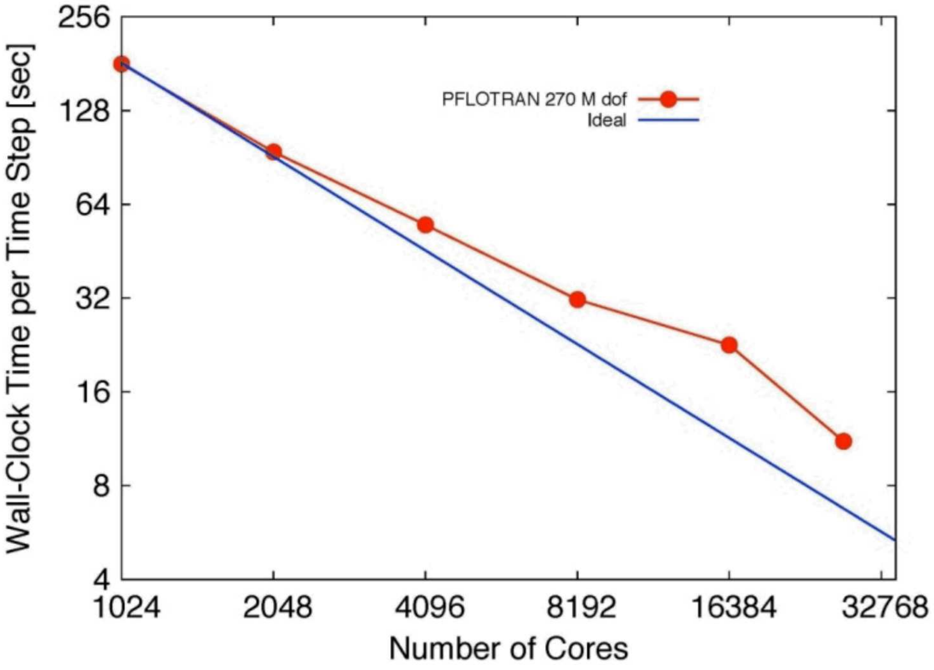
Open source license (GNU LGPL)

Object-oriented Fortran 2003/2008

Founded upon well-known (supported) open source libraries
- MPI, PETSc, HDF5, METIS/ParMETIS/CMake

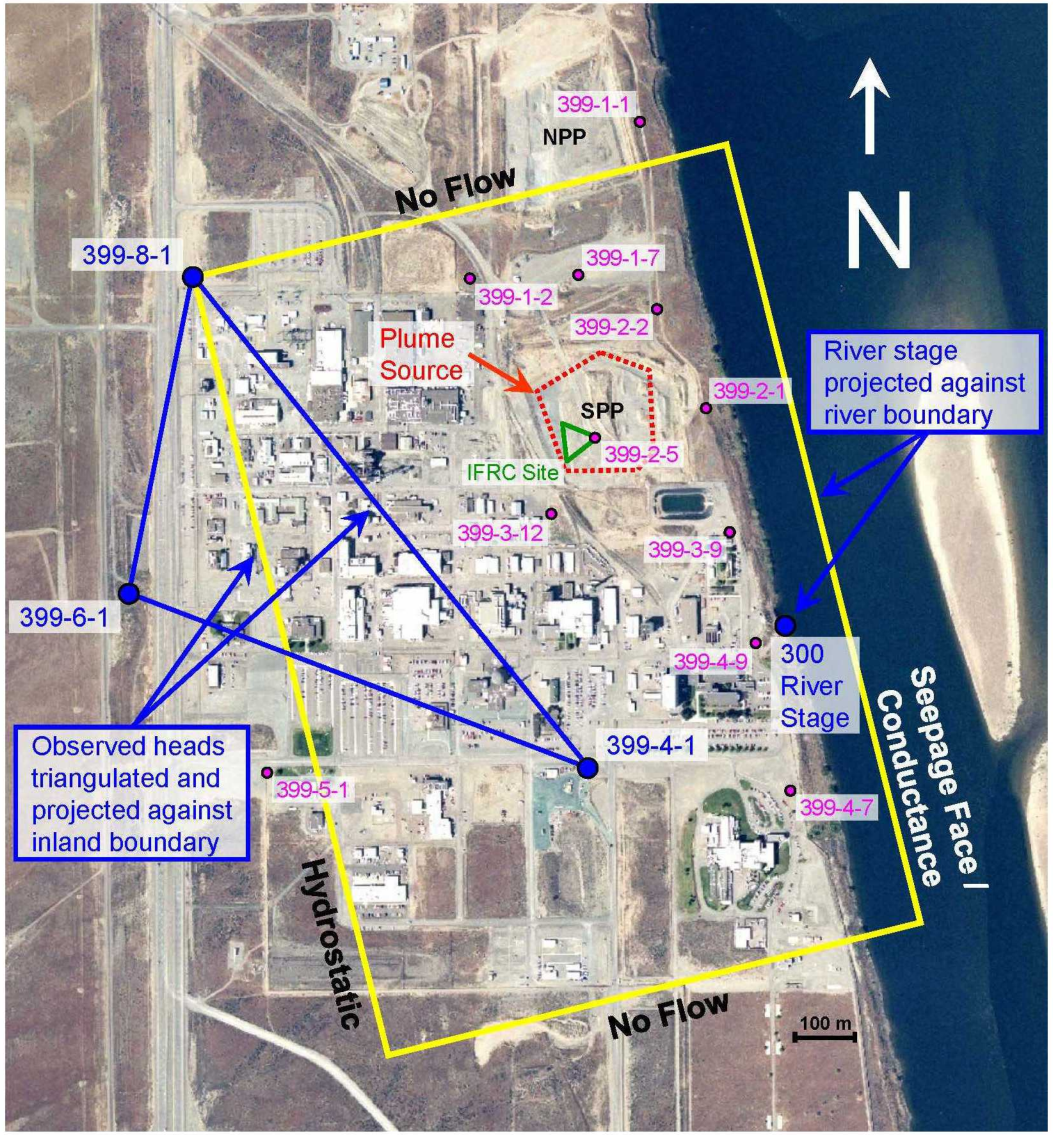
Demonstrated performance
- Maximum # processes: 262,144 (Jaguar supercomputer)
- Maximum problem size: 3.34 billion degrees of freedom
- Scales well to over 10K cores

More info.
- documentation.pflotran.org

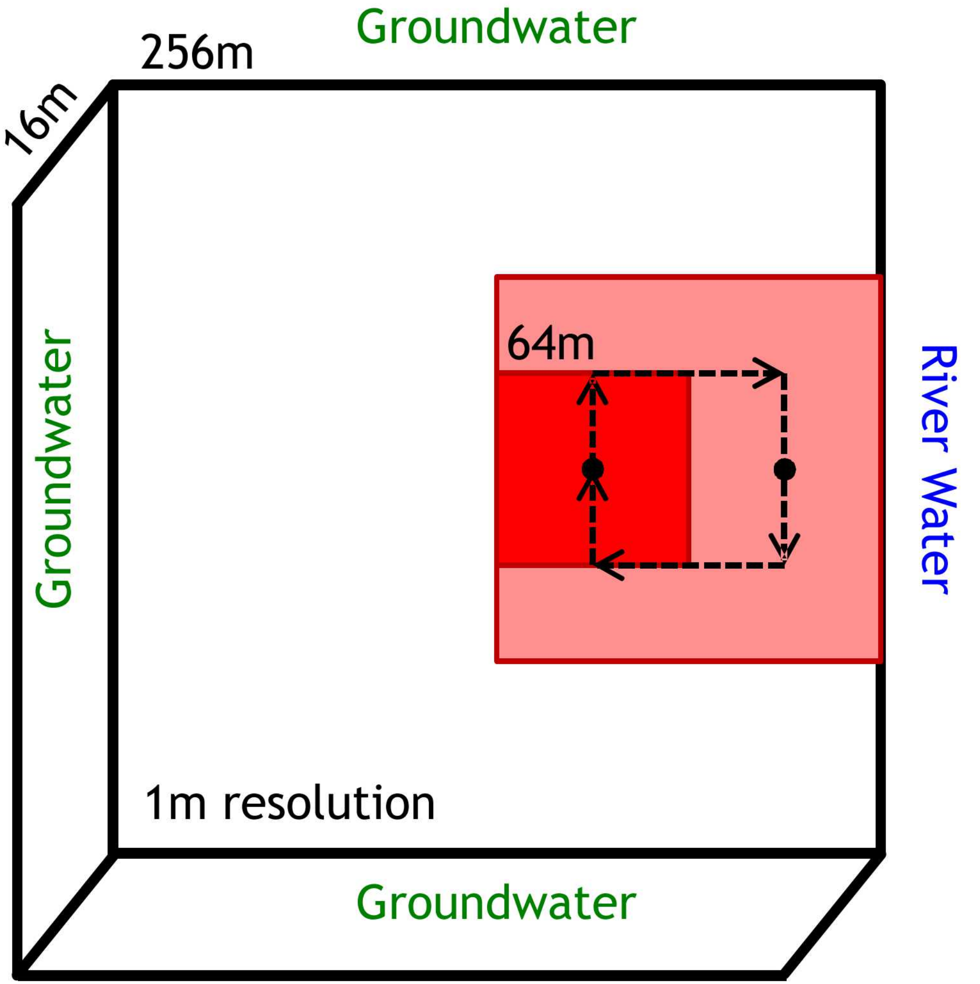


Hanford 300 Area Test Problem

Idealized Conceptual Model



Hammond, G.E. and P.C. Lichtner (2010) Field-Scale Modeling for the Natural Attenuation of Uranium at the Hanford 300 Area using High Performance Computing, Water Resources Research, 46, W09527, doi:10.1029/2009WR008819.



256 x 256 x 16 grid cells x 15 components = ~15.7M dof total

10 year simulation time

Run in parallel on 16 – 1024 processes (1M – 15K dof/process)

Geochemistry

15 primary aqueous species

- H^+, Ca^{2+}, $Cu^{2+,}$ $Mg^{2+,}$ UO_2^{2+}, K^+, Na^+, HCO_3^-, Cl^-, F^-, HPO_4^{2-}, NO_3^-, SO_4^{2-}, and 2 tracers

88 secondary aqueous species

- Dominant U(VI) species: $CaUO_2(CO_3)_3^{2-}$, $Ca_2UO_2(CO3)_{3(aq)}$

1 mineral

- Calcite

2 surface complexes and 1 surface site

- $>SOUO_2OH$, $>SOHOU_2CO_3$, $>SOH$

Groundwater and River Water Composition at Hanford 300 Area

	Groundwater†	River Water†
pH	7.6	7.8
Ionic Strength	6.88e-3	4.39e-4
Ca^{2+}	1.21e-3	4.50e-4
Mg^{2+}	5.10e-4	1.82e-4
HCO_3^-	2.57e-3	1.13e-3
K^+	1.55e-4	1.90e-5
Na^+	1.34e-3	5.12e-5
K_D*	5.56	62.37
Equilibrating Mineral	Calcite	N/A

† = equilibrated with sediment

K_D* = ratio of sorbed to aqueous mass [dimensionless K_D]

Governing Flow and Reactive Transport Equations

Flow

$$\frac{\partial}{\partial t}(\varphi s \rho) + \nabla \cdot \rho q = 0$$

$$q = -\frac{k k_r}{\mu} \nabla (p - \rho g z)$$

Reactive Transport

$$\frac{\partial}{\partial t}\left(\varphi s \Psi_j + \Psi_j^S\right) + \nabla \cdot \Omega_j = -\sum_m \nu_{jm}^{\mathrm{min}} I_m$$

$$\Omega_j = (q - \varphi s \tau D \nabla) \Psi_j$$

Total Aqueous Component Concentration

$$\Psi_j = C_j + \sum_i \nu_{ji}^{\mathrm{aq}} C_i$$

$$C_i = \frac{K_i}{\gamma_i} \prod_j \left(\gamma_j C_j\right)^{\nu_{ji}^{\mathrm{aq}}}$$

Total Sorbed Component Concentration

$$\Psi_j^S = \sum_{k\sigma} \nu_{jk}^{\mathrm{srf}} S_{k\sigma}$$

$$S_{k\sigma} = \frac{\omega_\sigma K_k Q_k}{1 + \sum_{k'} K_{k'} Q_{k'}}$$

$$Q_k = \prod_j \left(\gamma_j C_j\right)^{\nu_{jk}^{\mathrm{srf}}}$$

Mineral Precipitation-Dissolution

$$I_m = -k_m a_m \mathcal{P}_m (1 - K_m Q_m) \zeta_m$$

$$Q_m = \prod_j \left(\gamma_j C_j\right)^{\nu_{jm}^{\mathrm{min}}}$$

Prototype Dynamic K_D Model

Hanford 300 Area Dynamic K_D Model

$$\Psi_S = \phi s_l K_D \Psi$$

$$K_D = K_{D\,low} + \left(K_{D\,high} - K_{D\,low}\right) C_{river\ tracer}^{K_{D\,power}}$$

Ψ = aqueous concentration
Ψ_S = sorbed concentration
$C_{river\ tracer}$ = normalized tracer concentration (measure of river water fraction)
ϕ = porosity
s_l = liquid saturation
K_D = calculated ratio of sorbed to aqueous mass
$K_{D\,low}$, $K_{D\,high}$, $K_{D\,power}$ = parameters read from input deck

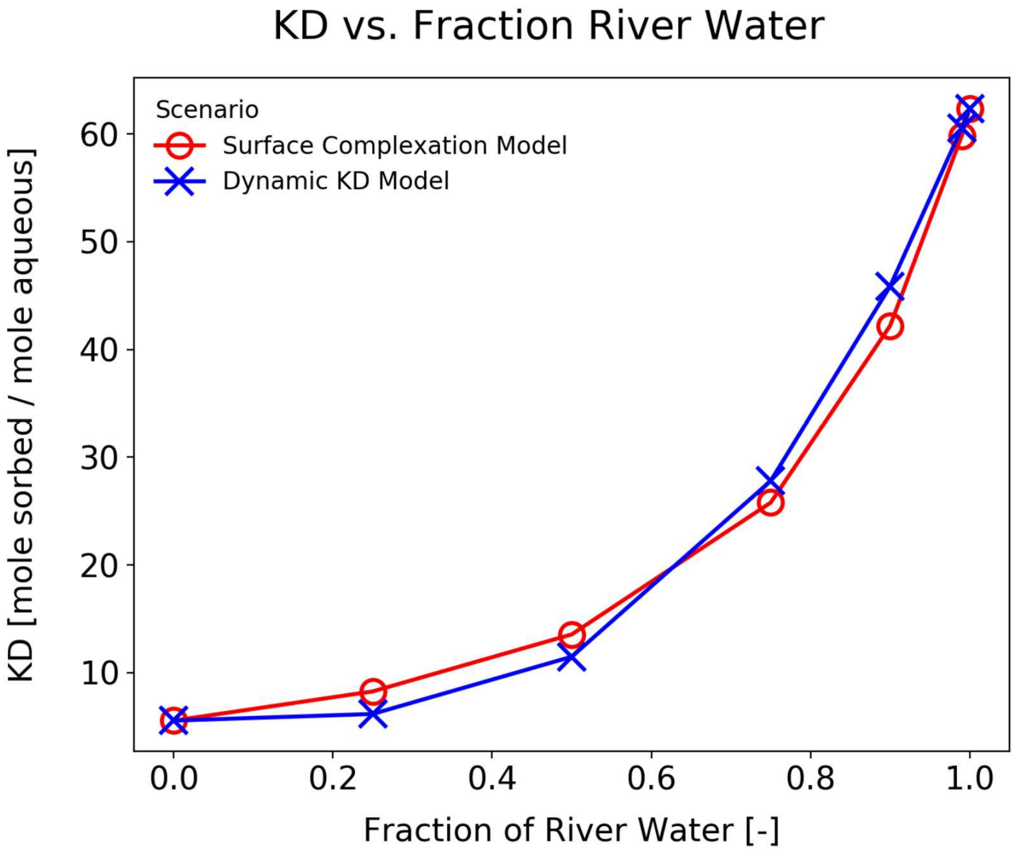
Hanford 300 Area Dynamic K_D Model

$$\Psi_S = \phi s_l K_D \Psi$$

$$K_D = K_{D_{low}} + \left(K_{D_{high}} - K_{D_{low}}\right) C_{river\ tracer}^{K_{D_{power}}}$$

$$K_D = 5.56 + (62.37 - 5.56) C_{river\ tracer}^{3.26}$$

Ψ = aqueous concentration
Ψ_S = sorbed concentration
$C_{river\ tracer}$ = normalized tracer concentration
ϕ = porosity
s_l = liquid saturation
K_D = calculated ratio of sorbed to aqueous mass
$K_{D_{low}}$, $K_{D_{high}}$, $K_{D_{power}}$ = parameters read from input deck


KD vs. Fraction River Water

Scenarios for Comparison

Sorption Model	Prescribed Uniform Flow		Heterogeneous Flow Field	
Constant K_D	Operator Split	Global Implicit	Operator Split	Global Implicit
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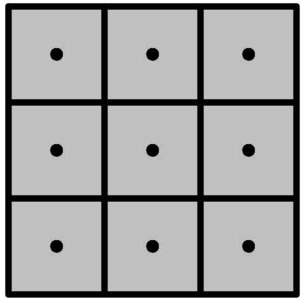
Prescribed Uniform Flow = Reactive transport only in a uniform velocity field that changes over time (i.e. no flow calculation).

Heterogeneous Flow Field = Flow and reactive transport in a heterogeneous permeability field with dynamic piezometric head gradients that change over time.

Global Implicit vs. Operator Split Coupling

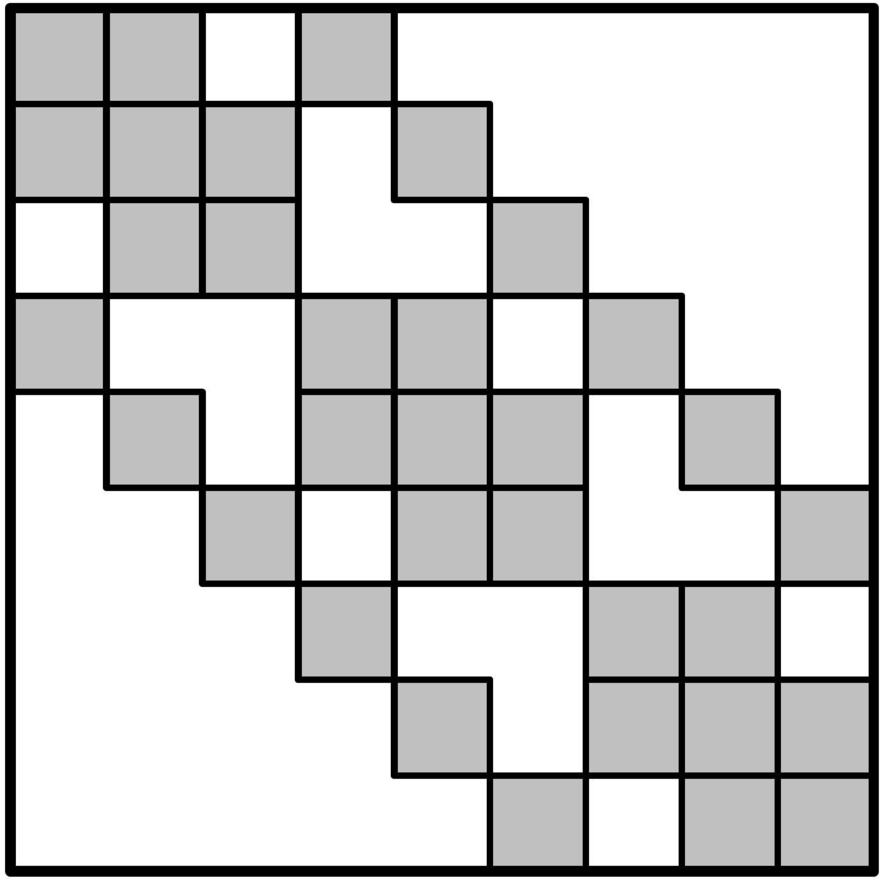


9 cells
3 chemical components

For each timestep:

Global Implicit Coupling

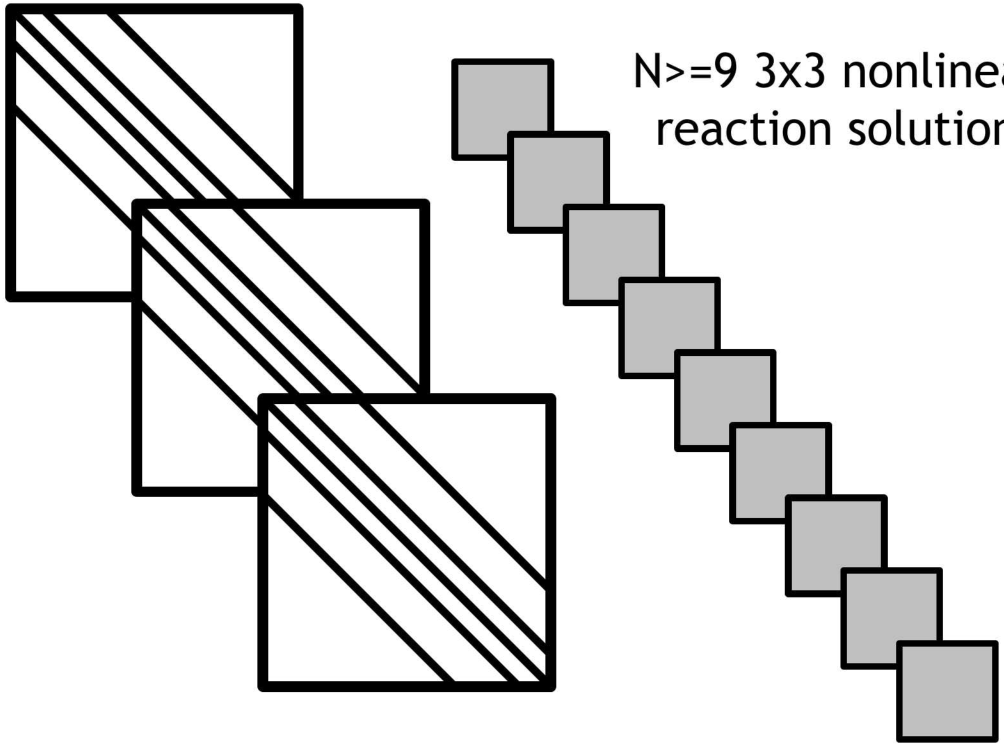
N>=1 27x27 coupled nonlinear solutions



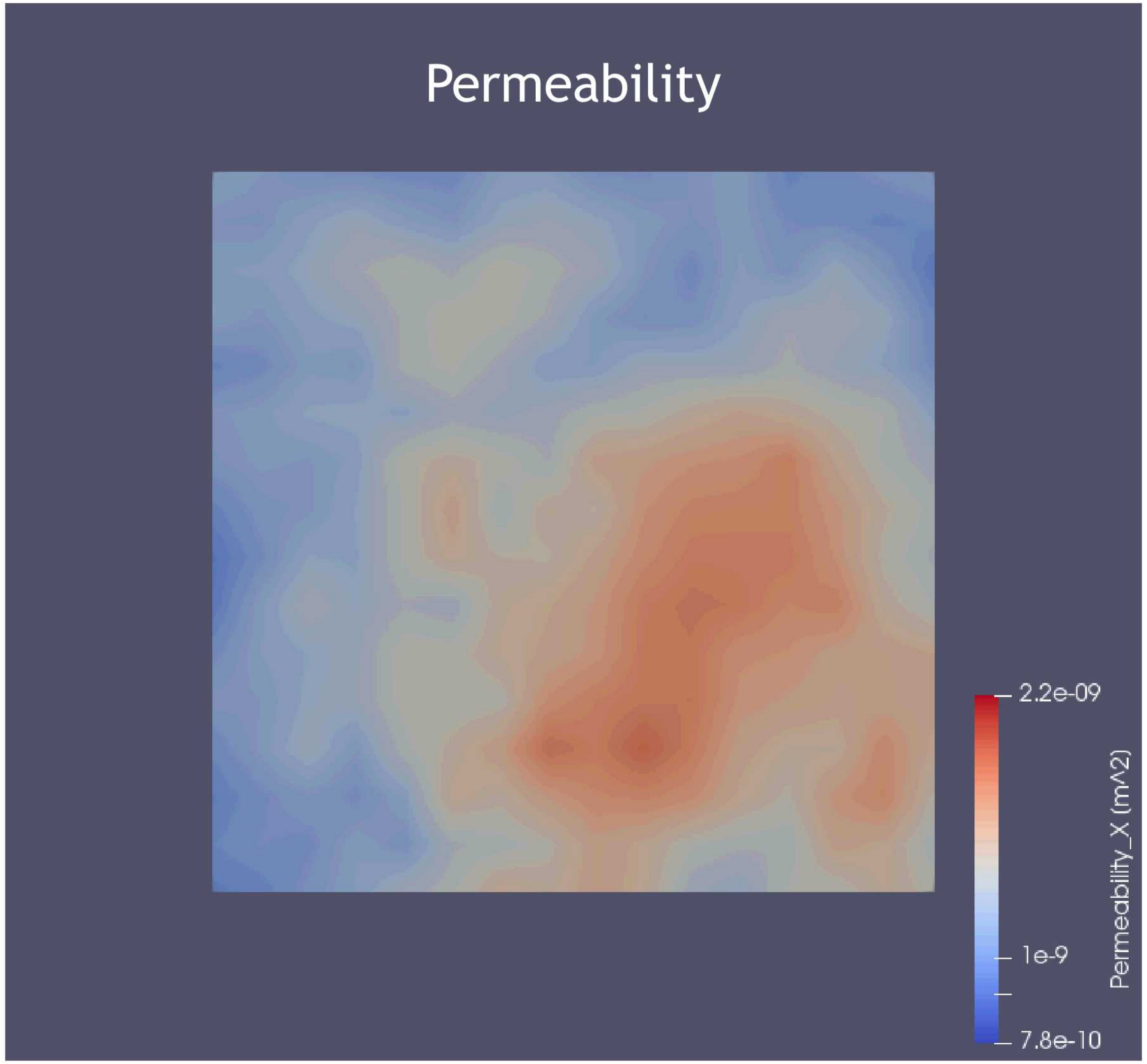
Operator Split Coupling

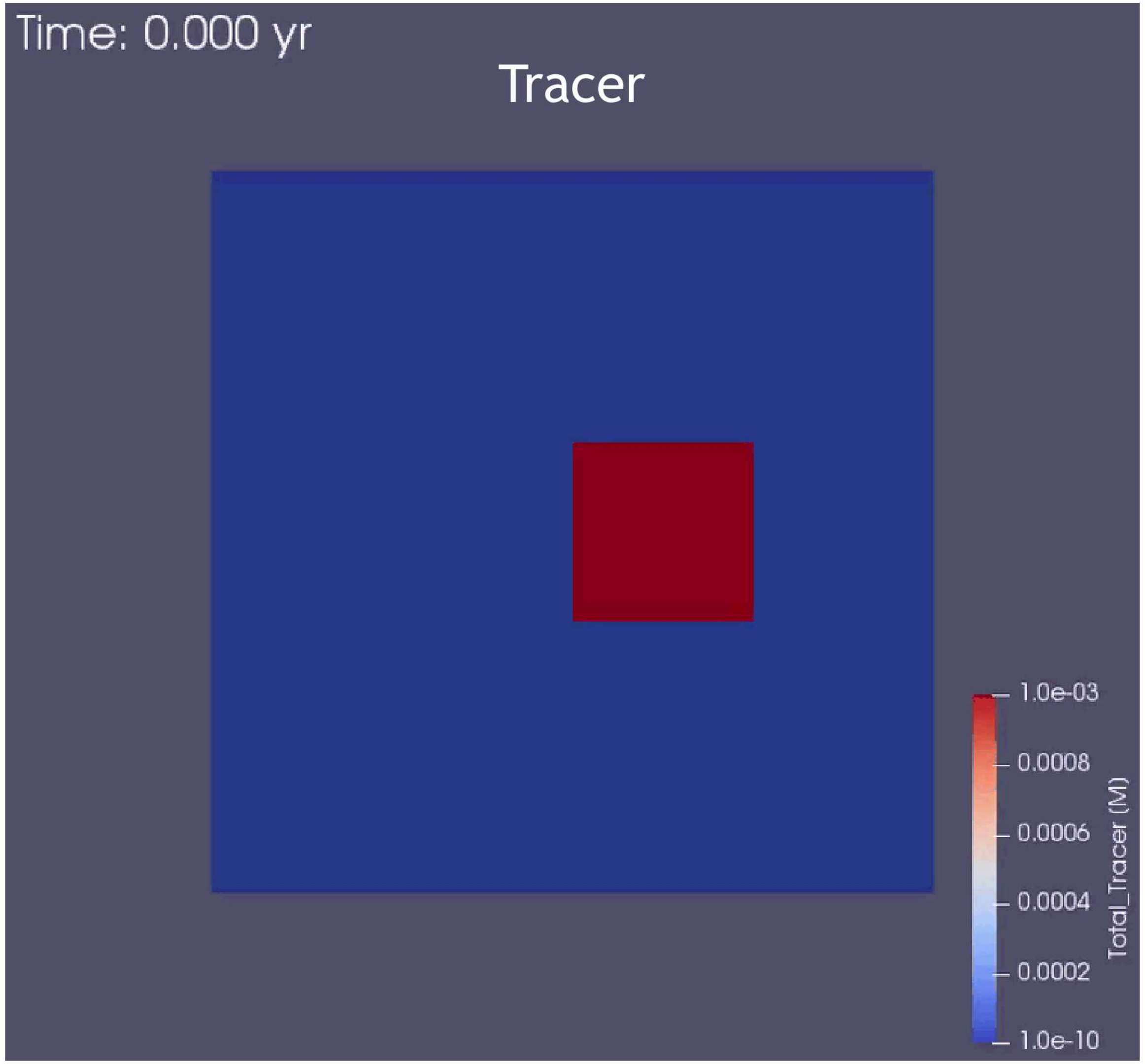
3 9x9 sparse linear
transport solutions

N>=9 3x3 nonlinear
reaction solutions



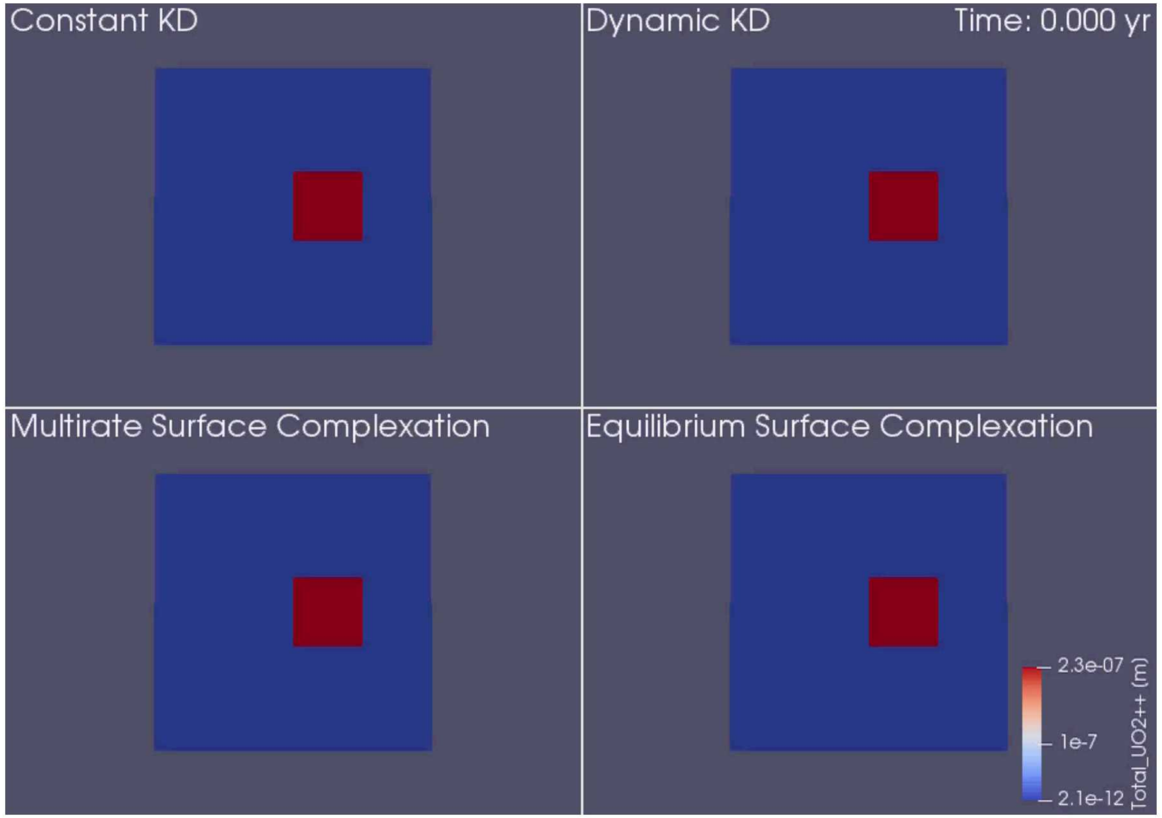
Tracer Animation in Heterogeneous Flow Field



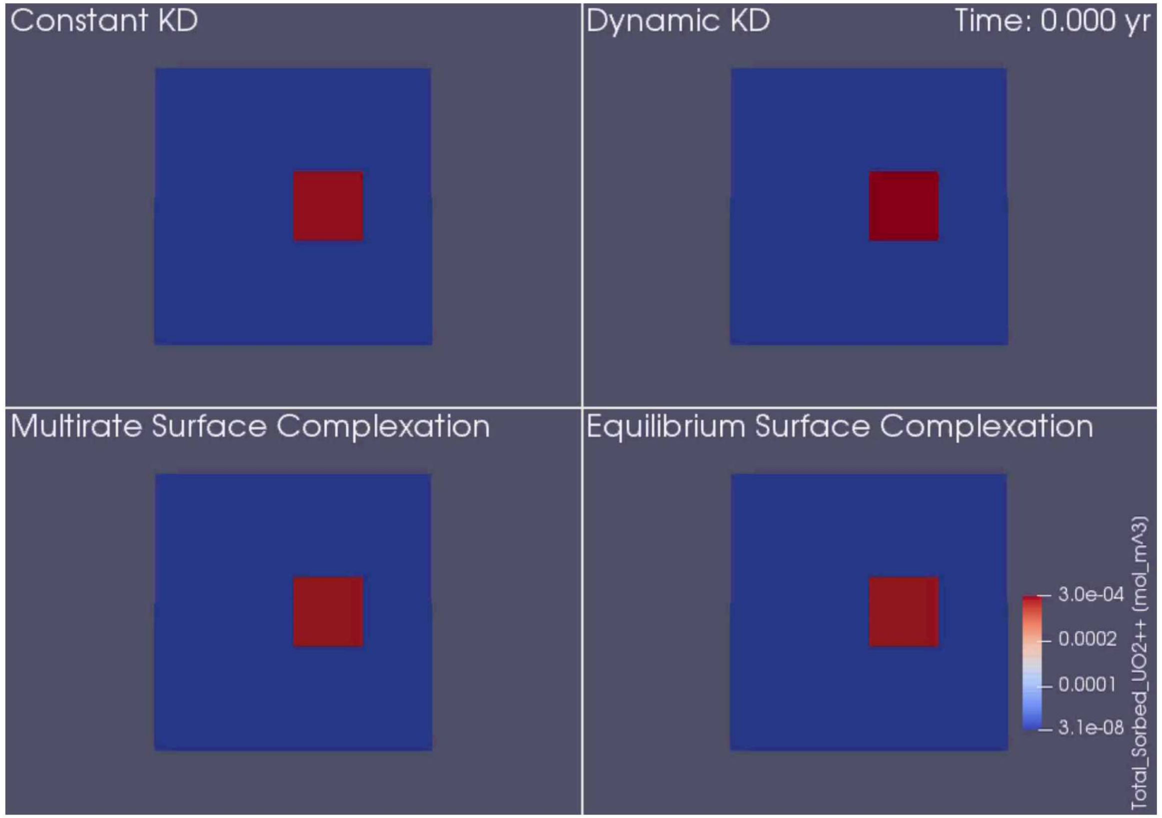


Animations of Aqueous and Sorbed UO_2^{++}

Aqueous UO_2^{++}

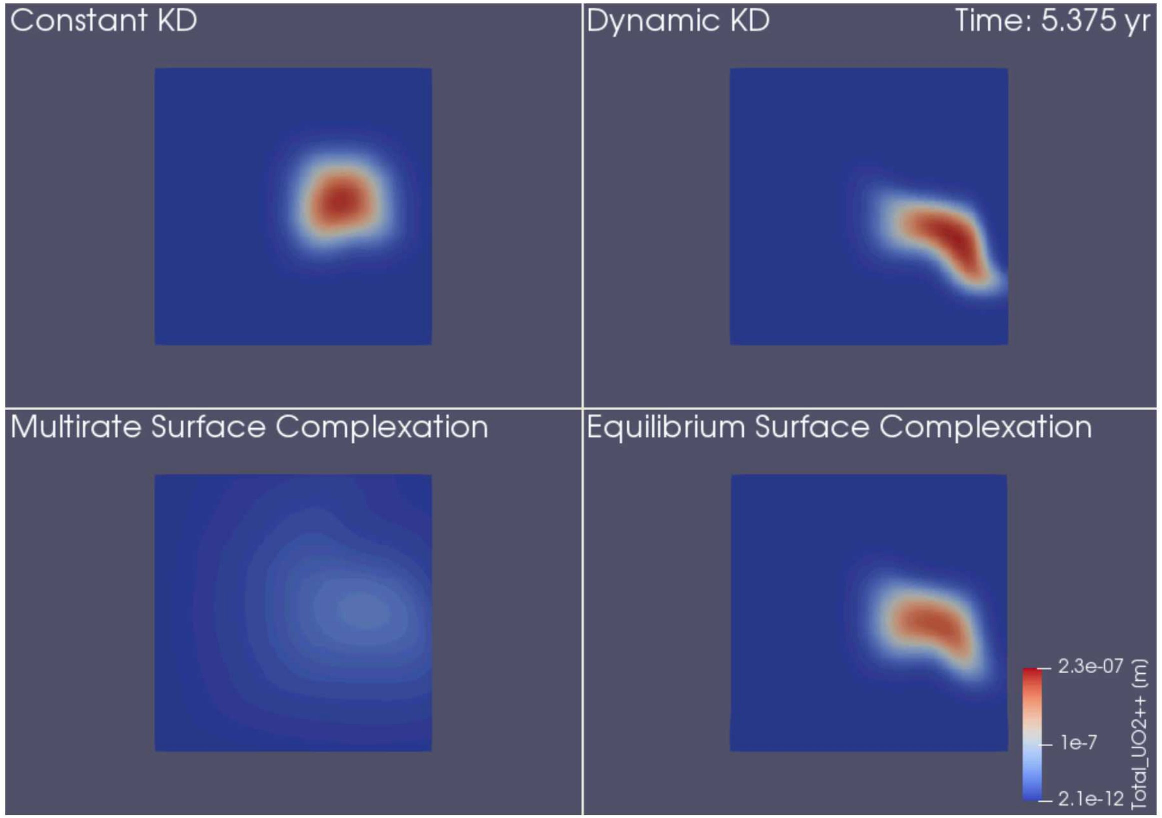


Sorbed UO_2^{++}

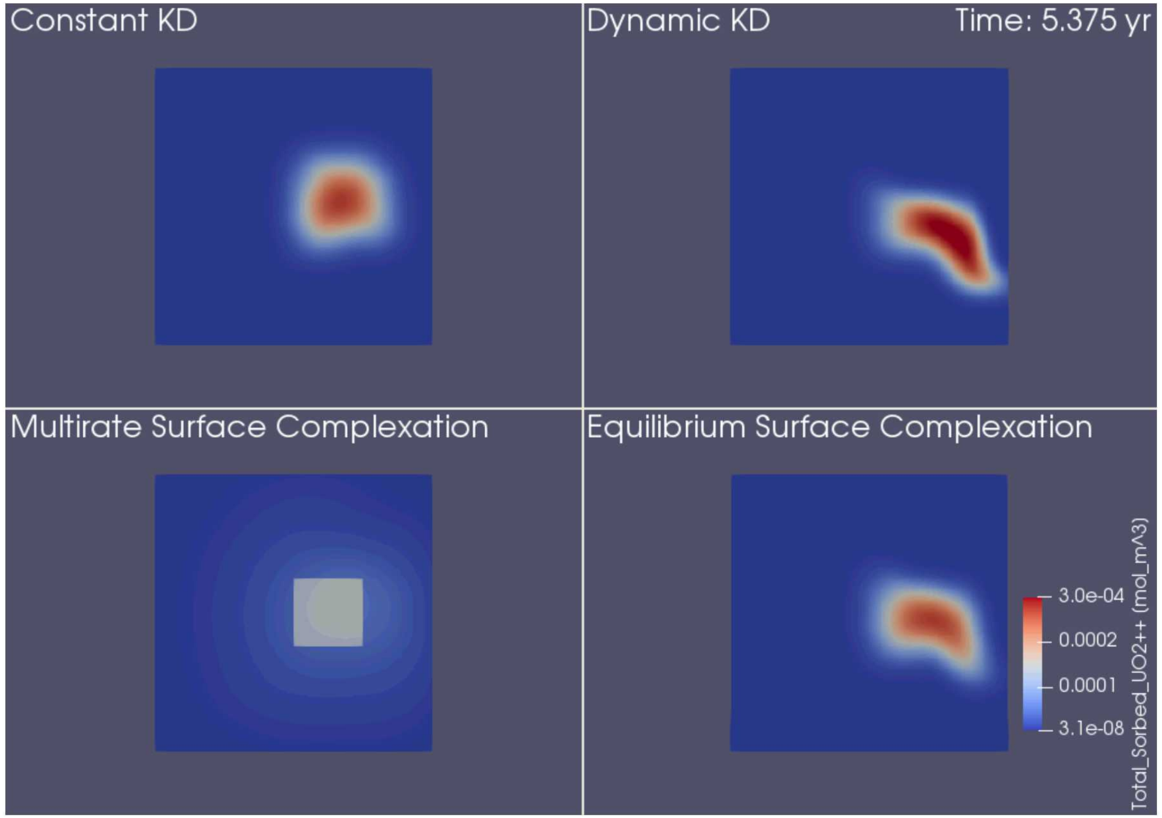


Snapshots of Aqueous and Sorbed UO_2^{++} at 5.375 Years

Aqueous UO_2^{++}



Sorbed UO_2^{++}

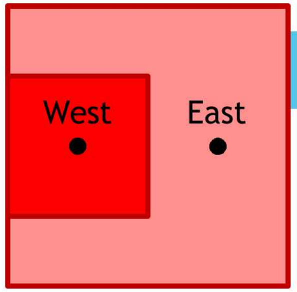


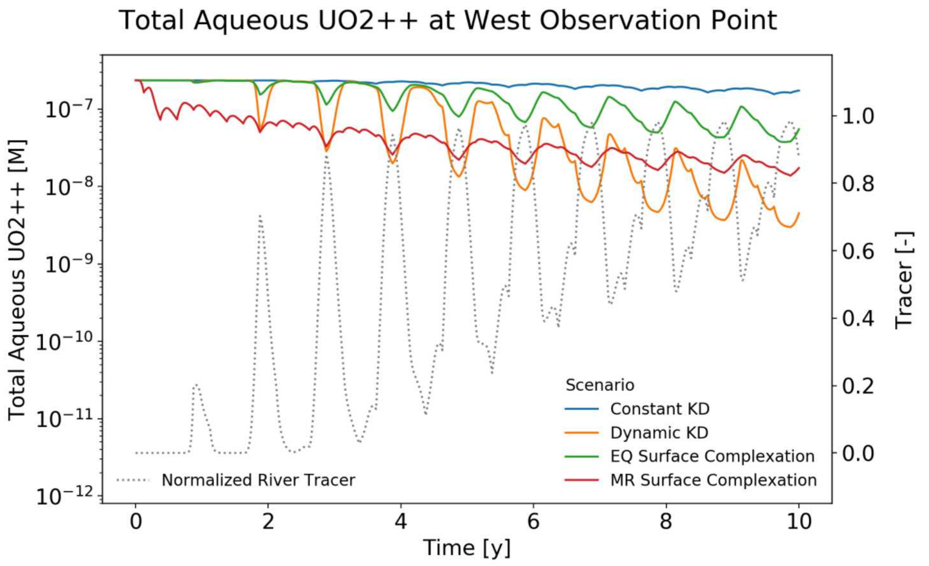
Parallel and Algorithmic Speedup Results

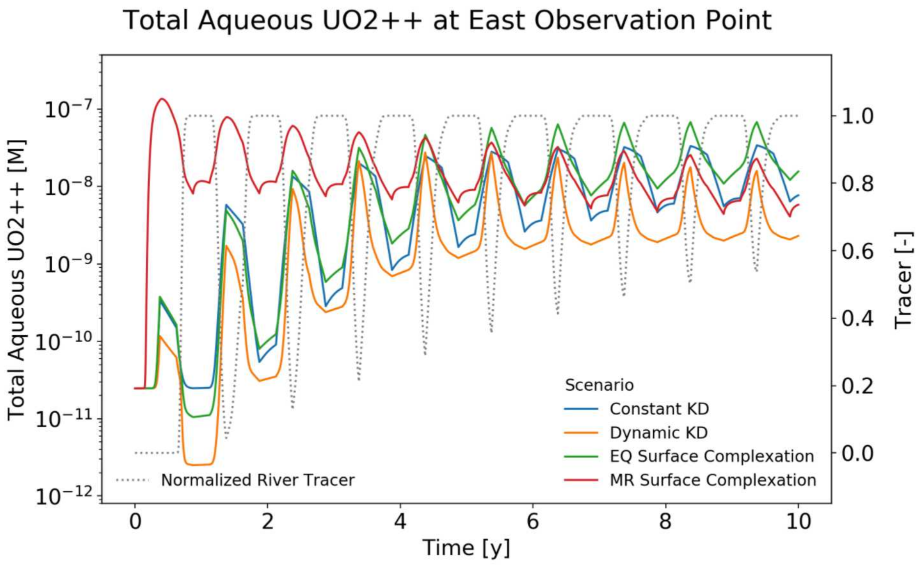
What is the maximum speedup obtainable through parallel processing?

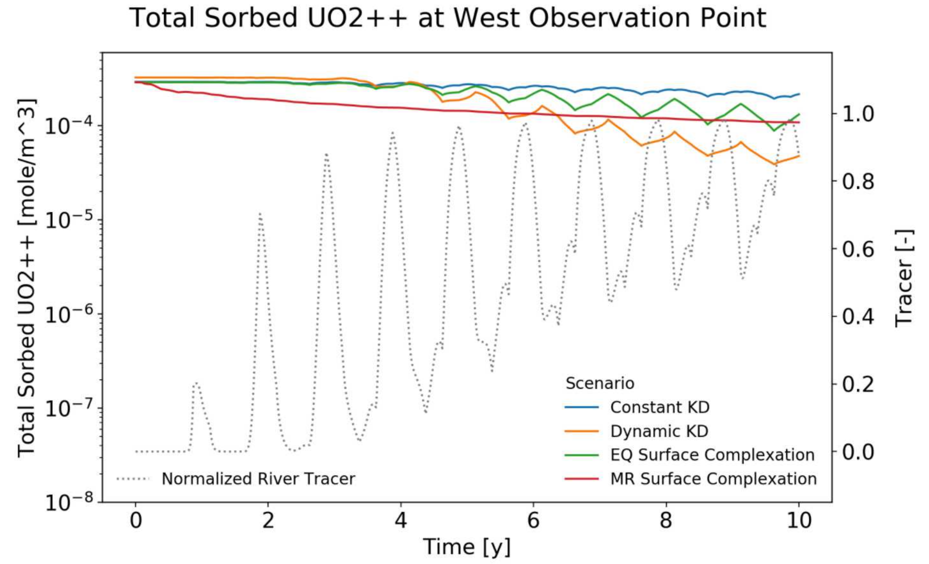
What is the maximum speedup obtainable through simplification of chemistry?

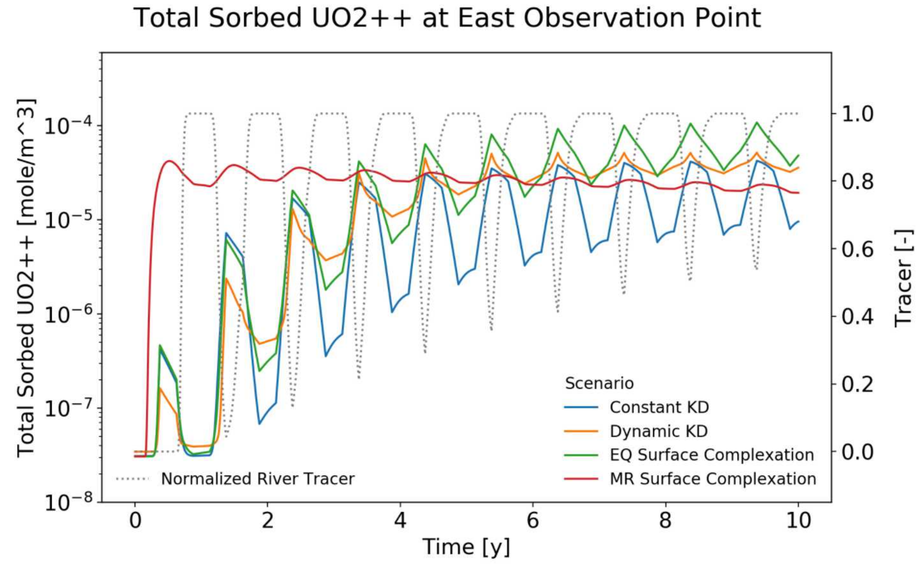
Breakthrough of Aqueous and Sorbed UO_2^{++} at Observation Points



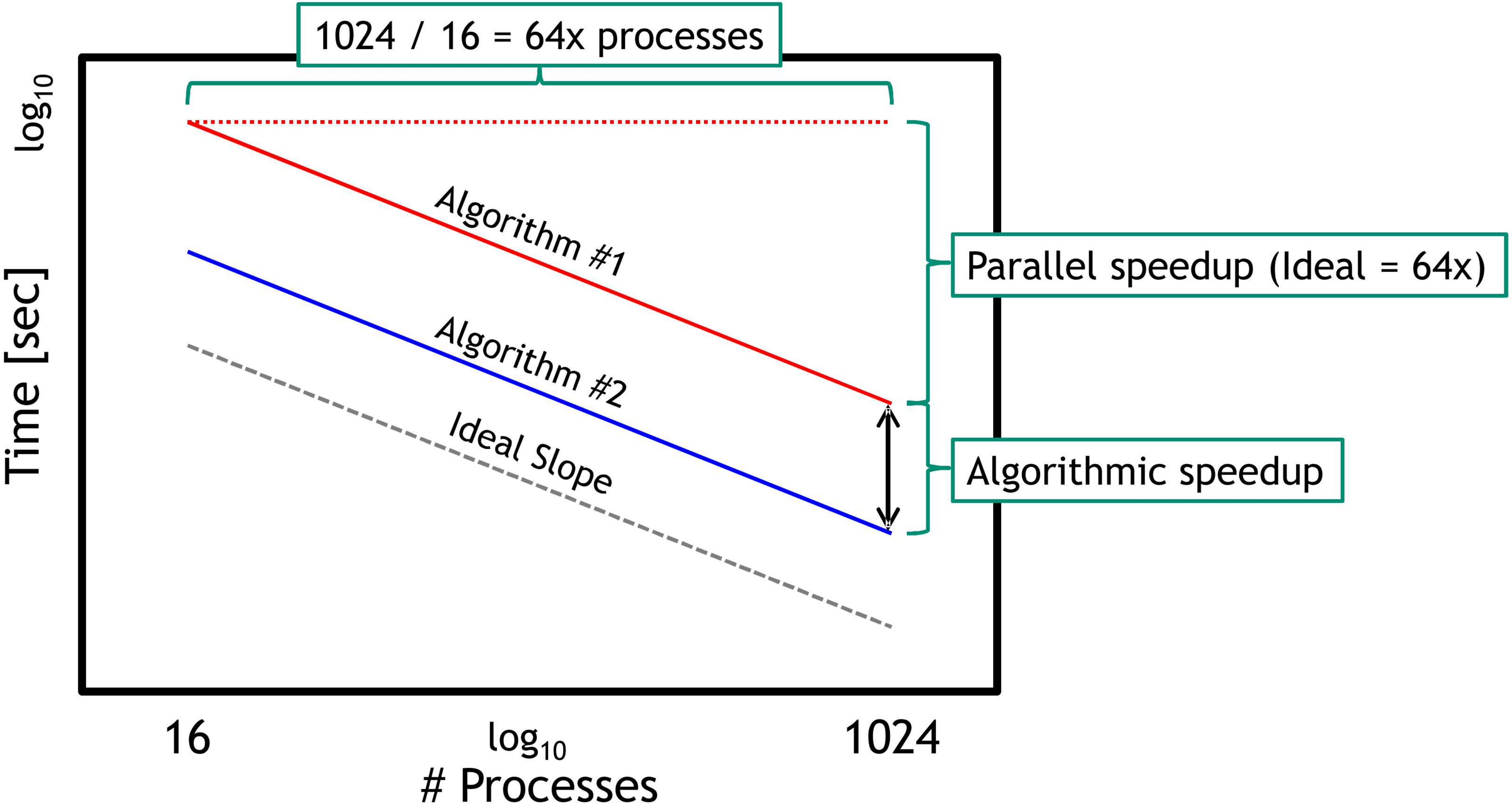








Schematic of Speedup Results

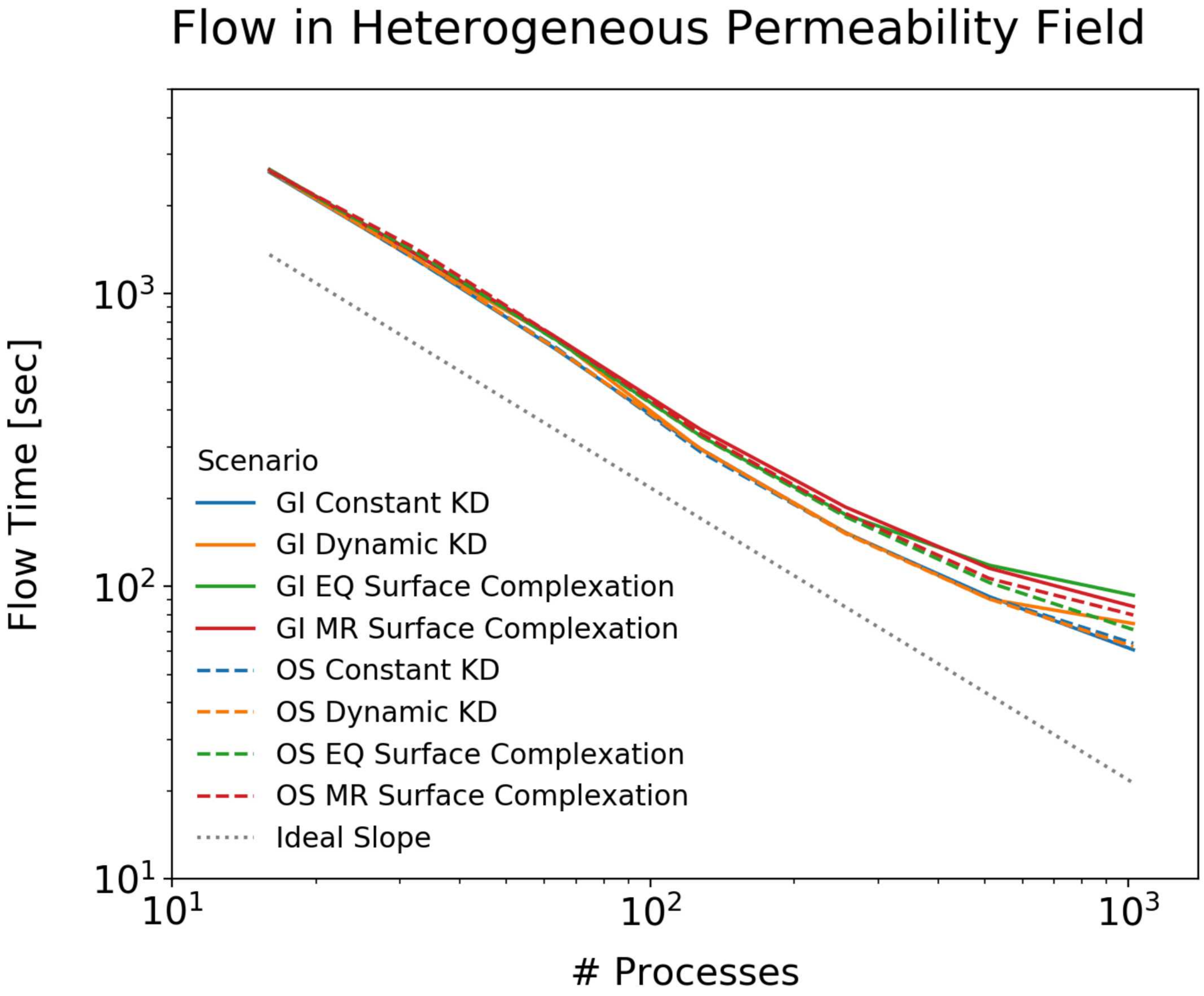


1024 / 16 = 64x processes

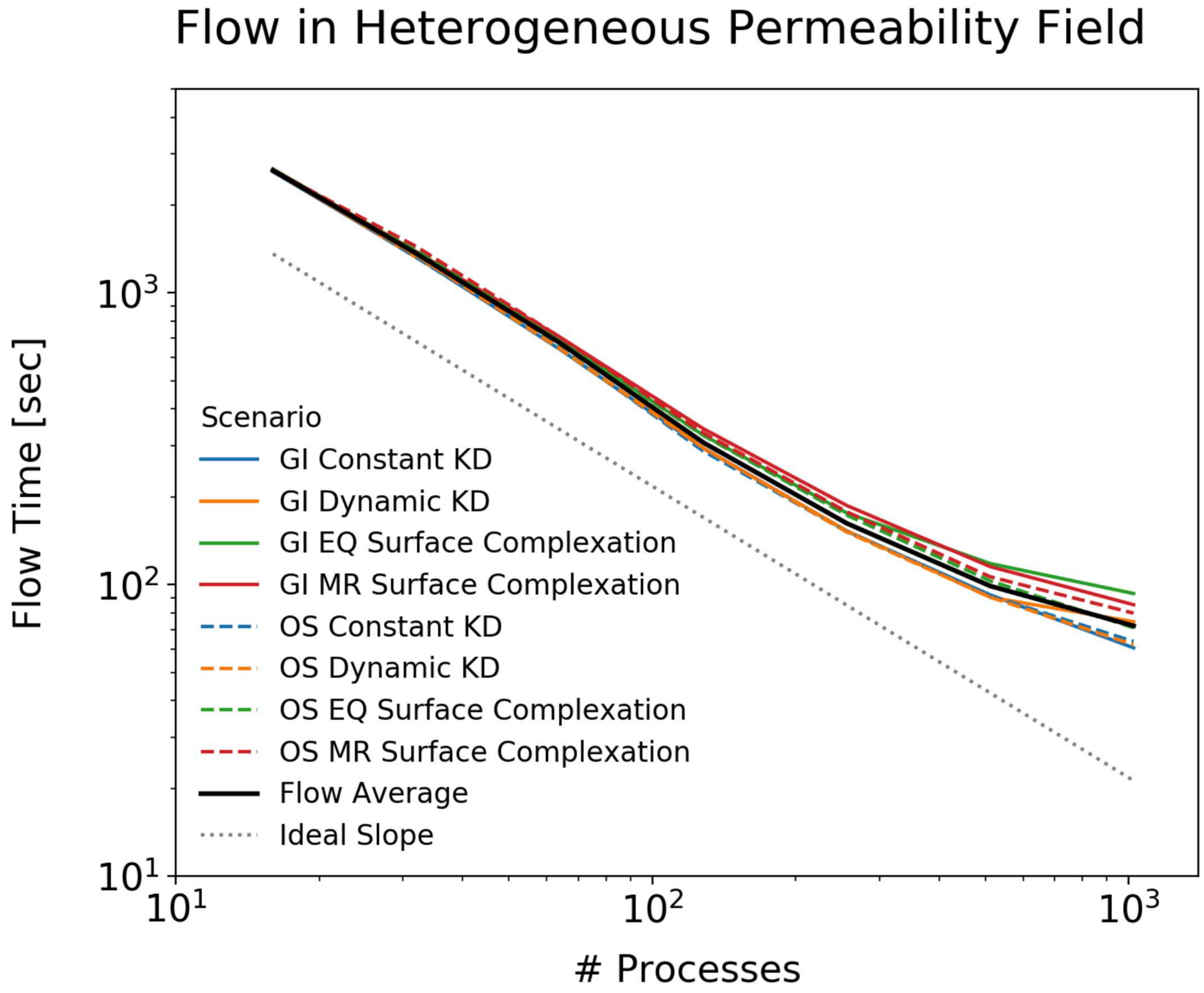
Parallel speedup (Ideal = 64x)

Algorithmic speedup

Flow Solution Times

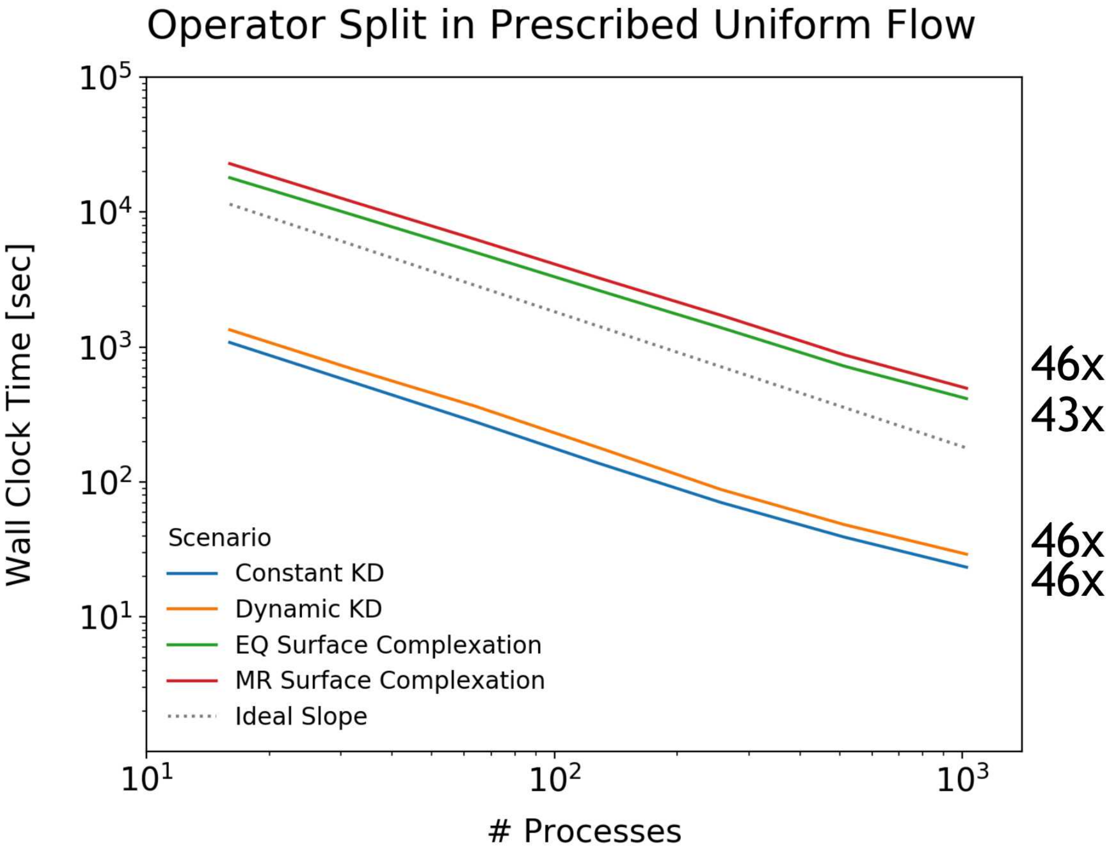


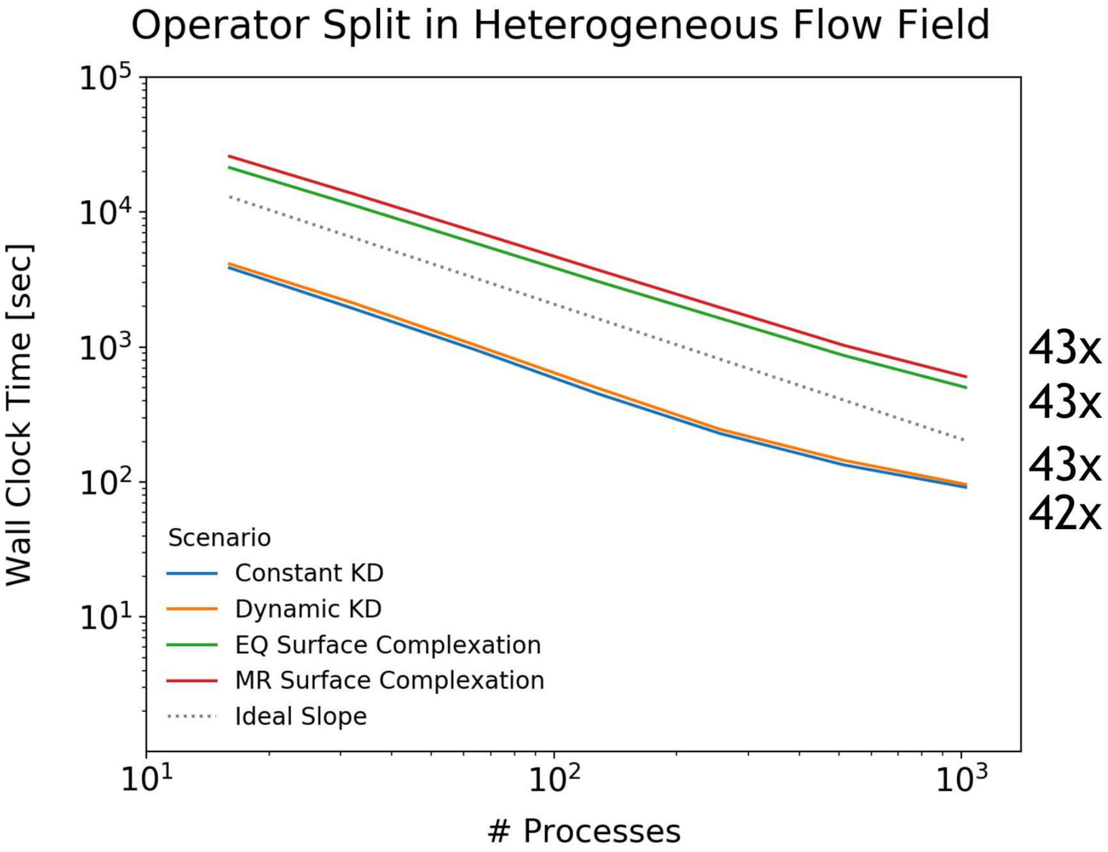
Flow Solution Times



Bounds of Speedup Due to Parallel Processing: Operator Split

Parallel Speedup

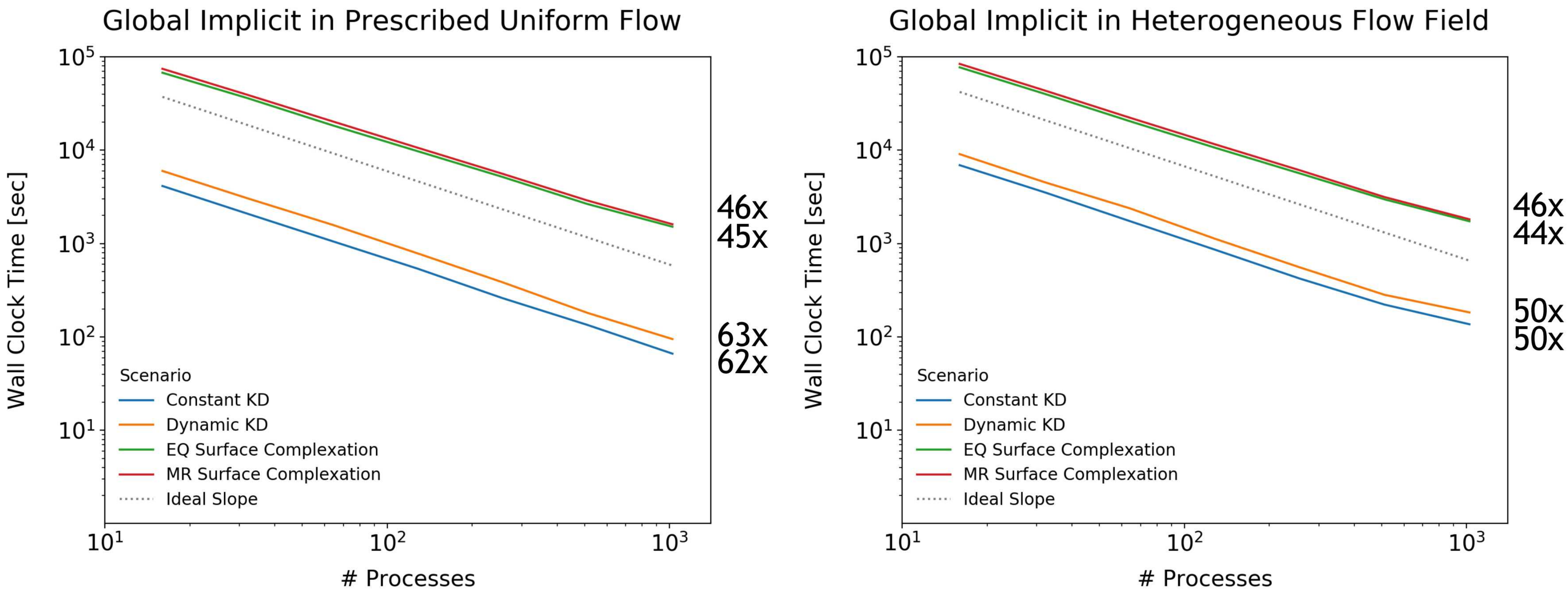




Ideal Speedup = 64x

Bounds of Speedup Due to Parallel Processing: Global Implicit

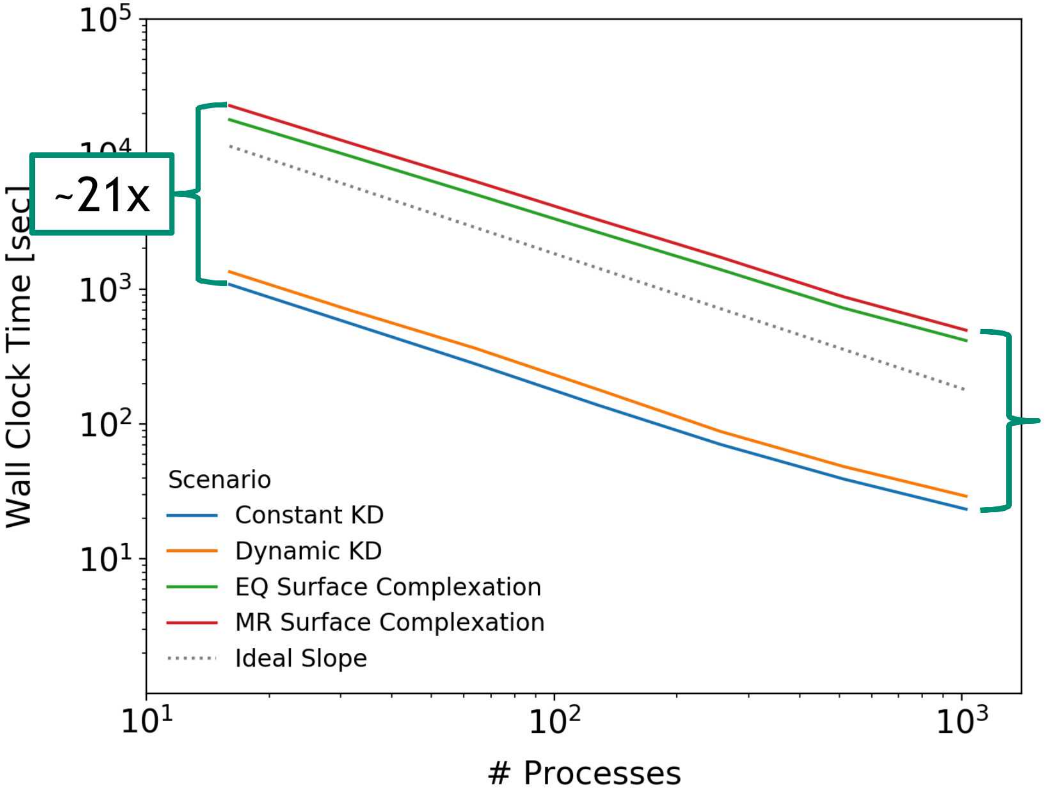
Parallel Speedup



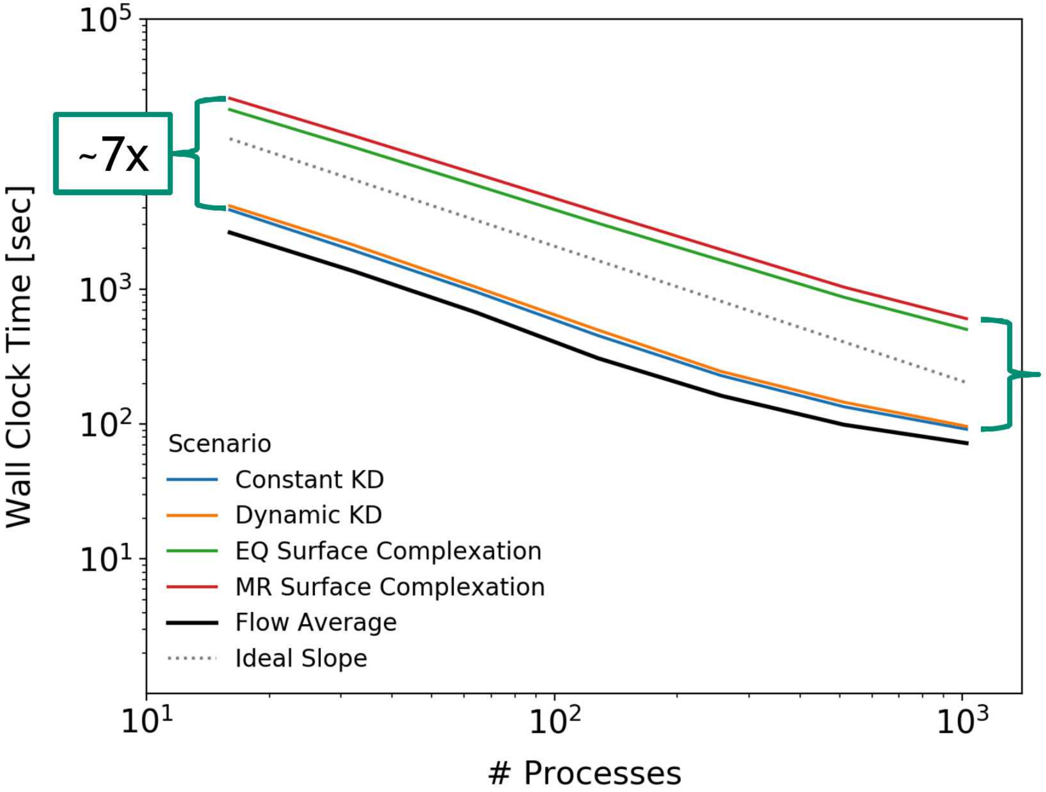
Ideal Speedup = 64x

Operator-Split: Prescribed Uniform Flow vs. Heterogeneous Flow Field

Algorithmic Speedup


Operator Split in Prescribed Uniform Flow

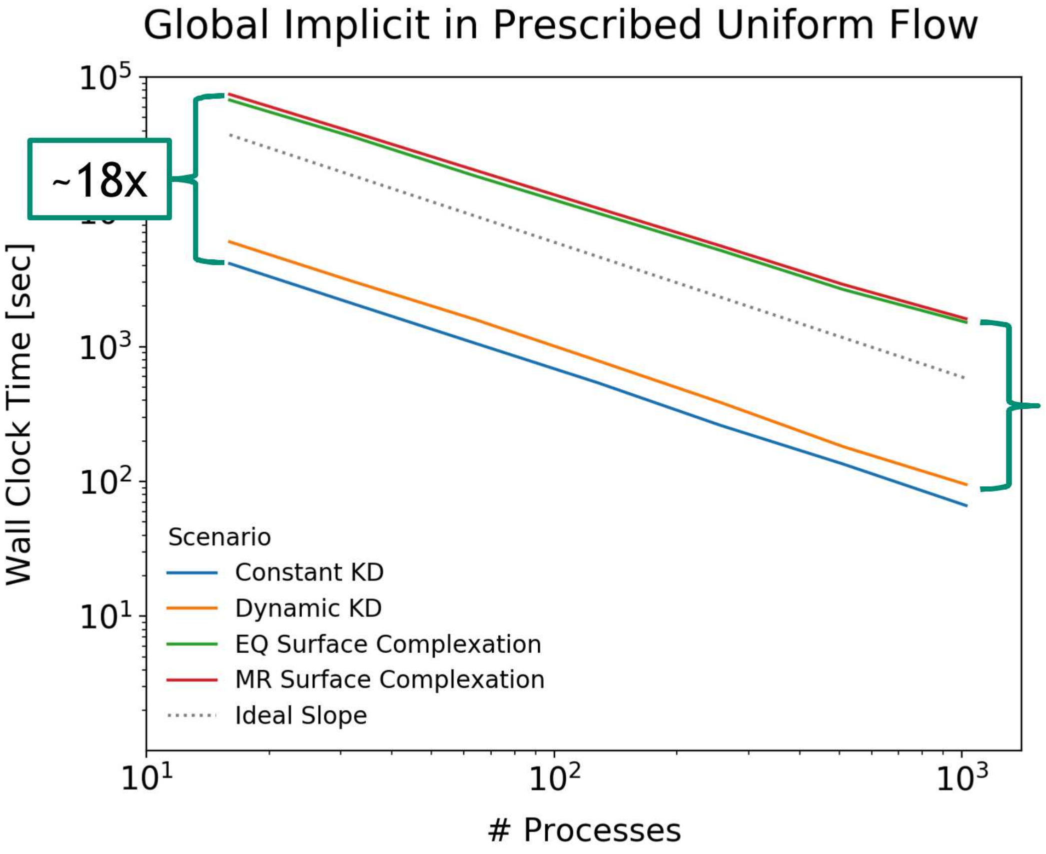
~21x

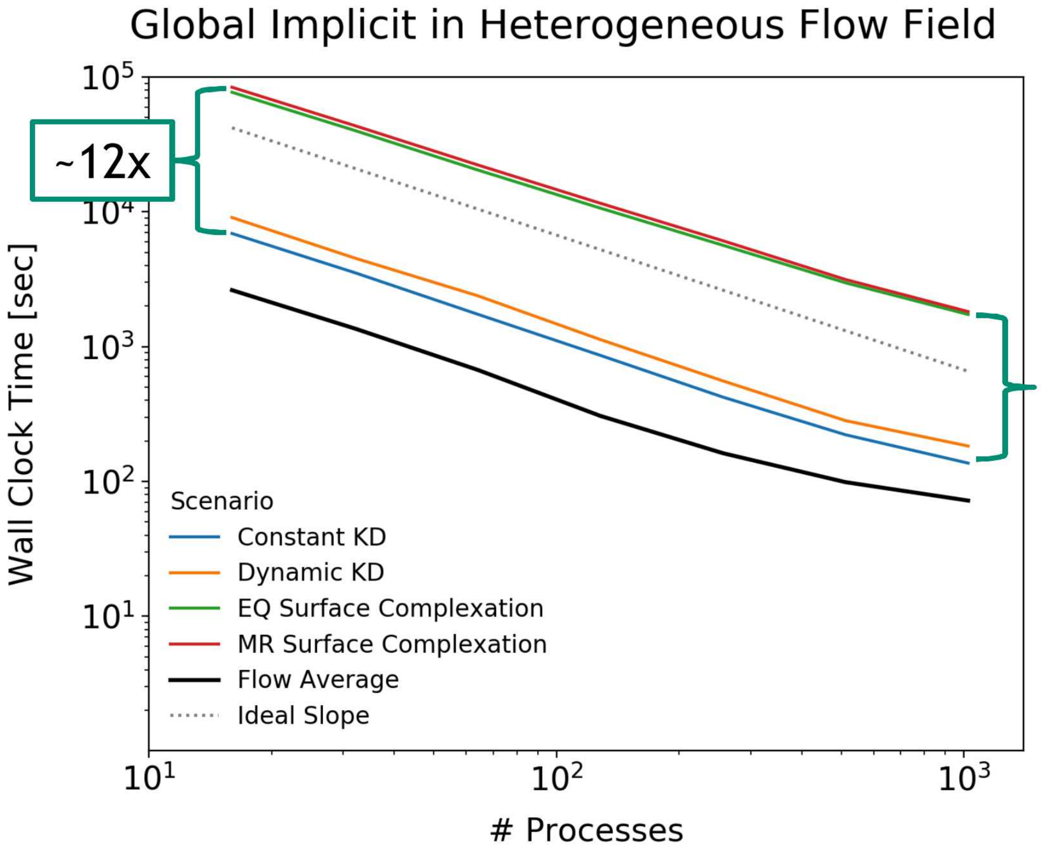

Operator Split in Heterogeneous Flow Field

~7x

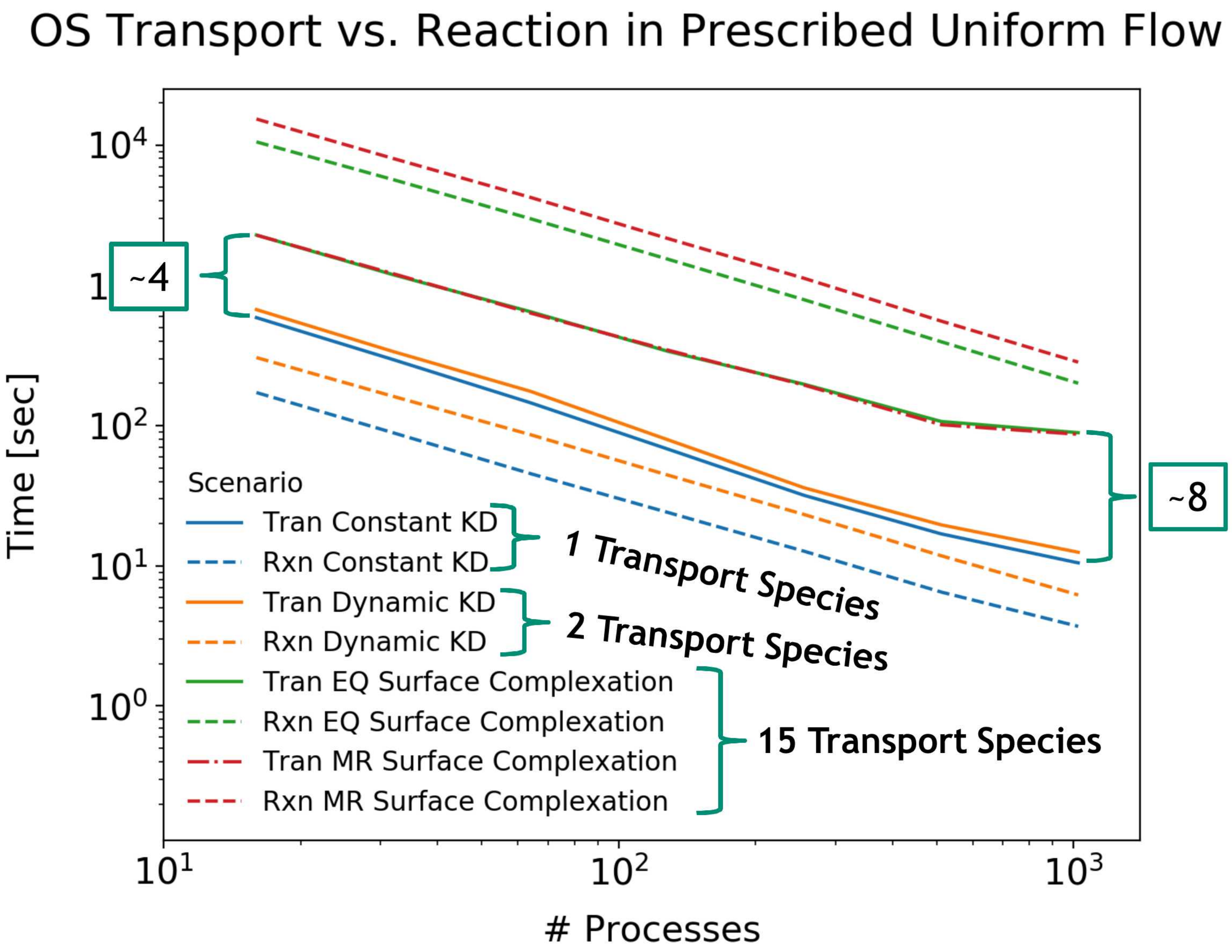
Global Implicit: Prescribed Uniform Flow vs. Heterogeneous Flow Field

Algorithmic Speedup





Transport vs. Reaction



~4

~8

1 Transport Species

2 Transport Species

15 Transport Species

Application of Amdahl's Law to Maximum Speedup in Reactive Transport

$$T_{total} = T_{transport} + T_{reaction}$$

$$T_{reaction} \rightarrow 0: T_{min} = T_{transport}$$

$$T_{reaction} = 0.9\, T_{total}$$

$$T_{min} = T_{transport} = 0.1\, T_{total}$$

Maximum Possible Speedup = 10x

Conclusions

For representative surface complexation problem (~1M grid cells × 15 chemical components = ~15.7M dof total)

Maximum speedup (efficiency) due to parallel processing:

Ideal = 64 (100%)

	Operator Split	Global Implicit
Specified Uniform Flow	46.3 (72%)	63.1 (99%)
Heterogeneous Flow Field	43.0 (67%)	50.5 (79%)

Maximum speedup due to simplified chemistry:

	Operator Split	Global Implicit
Specified Uniform Flow	~21	~18
Heterogeneous Flow Field	~7	~12

Maximum speedup due to both parallel processing and simplified chemistry

	Operator Split	Global Implicit
Specified Uniform Flow	977	1122
Heterogeneous Flow Field	283	613