Intrinsic Parallelism and Implementation of a High-Performance Hydrobiogeochemical Model

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What is HydroBioGeoChem 123D (HBGC123D)?

- Models in one, two and three dimensions.
- Kinetic and equilibrium reactions in variably saturated media.
- Coupled monod kinetics for biochemistry reactions.
- Non-isothermal hydrologic transport for temperature dependent density and solute reactants.
- Documentation and software available online at `http://hbgc.esd.ornl.gov/`

Numerical approach

- A Lagrangian-Eulerian finite element method is used to solve the heat transfer and transport equations.
- Uses special line elements in one dimensions, triangles and quadrilaterals in two dimensions, hexahedral (6 faces), pentahedral (5 faces) and tetrahedral (4 faces) elements in three dimensions.
- HBGC123D is flexible in accepting an unstructured mesh (list of elements).
- Option for upwind weighted finite element method for Eulerian transport.
- Option for backward particle tracking in Lagrangian transport.
- Gradient calculation at nodal values is by assembly of basis functions and lumped mass matrix.

Shared memory parallel implementation

- SGI compiler directives for shared memory multiprocessors system.
- Relatively easy to perform. Selectively parallelize only time consuming kernels.
- Requires care in identifying variables with local, shared or reduction attributes.
- Requires extra temporary storage per thread.
- Dynamic load balancing is possible.

Distributed memory parallel implementation

- Distributed memory version still under development and testing.
- ‘All or nothing’ effort.
- Simple decomposition and distribute work by assigning *contiguous* blocks of nodes to processors.
- Modify time consuming loops to range over subset of nodes (or elements).
- Replicate arrays to easily implement Lagrangian particle tracking.
- Another approach requires a “ghost region” and time step reduced to ensure no particle can escape subdomain.

Chemistry module

- Chemistry module based on hydrobiogeochemistry work by Prof George Yeh at Penn State University.
- Computation based solely on conditions at node. Same chemistry module for one, two and three dimensions.
- Equilibrium reactions model as solution of system of non-linear algebraic equations.
- Newton’s method with explicit Jacobian matrix is used to enhance convergence.
- Very ill-conditioned matrices may require full (row and column) pivoting in LU decomposition.
- Kinetic reactions can handled in a coupled fashion with solute transport.

Nonlinear iteration

- (1) Handle heat transport.
- (2) Handle transport for all aqueous (mobile) chemical components and kinetically controlled species.
- (3) Calculate equilibrium chemistry in a node by node manner.
- Advance to next time step if operator splitting option is used; otherwise iterate on Steps (2) and (3) until convergence to self-consistency.

Element assembly for Eulerian transport

- Elements are grouped (colored) into maximal independent sets. Two elements are *dependent* if they share at least one common node. Two dependent elements must be assigned distinct colors.
- Elements within an independent set can be assembled and added to the global sparse matrix without conflict.
- Setting up source, sink and boundary conditions still performed in serial.
- BiCGSTAB or Conjugate Gradients preconditioned with simple diagonal scaling is available to solve sparse linear system in parallel. Other options include band solver, Krylov iterative method preconditioned by SSOR, ILU, and matrix polynomials.

Microbiological and chemical reactions

- Benchmark problem for reactive transport by Valocchi and Tebes (1997).
- Simulation of biodegradation in a lab scale column.
- The problem includes these processes:
  - advective/dispersive transport
  - kinetic adsorption/desorption
  - equilibrium aqueous complexation and biodegradation
  - 3D simulation with 100 elements and 404 nodes on a uniform grid
  - 7 components, 14 complexed species, 2 kinetically adsorbed species, 1 microbial species

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Nonlinear algebraic equations

- Depending on the complexity of reactions and number of species, the chemistry module commonly is the most expensive component.
- Each node requires $O(m^3)$ (m is related to number of species) operations in LU factorization of Jacobian matrix in solving the nonlinear equations.
- This is highly parallel since each reaction depends solely on condition at node. Totally decoupled after transport.

Lagrangian particle tracking

- Independent particle tracking can proceed in parallel.
- Precomputes neighbor connectivity (which element shares a face).
- In one and three dimensions, a trajectory within each element is assumed to be a simple straight line. This greatly speeds up the computation and also leads to simpler coding.
- In two dimensions, another option subdivides an element for more accurate tracking of the trajectory as a continuous sequence of piecewise linear segments.
- Extra care is needed for handling trajectories near corner nodes. Tetrahedral and pentahedral elements with planar faces should be used to avoid non-planar faces in hexahedral bricks.

nproc	chemistry	Eulerian(assembly)	Lagrangian	grad	total
serial	4.8s	1.2s (1.1s)	0.3s	1.4s	7.1s
1	4.7s	1.2s (1.1s)	0.3s	1.4s	7.1s
2	2.6s	0.7s (0.6s)	0.2s	0.8s	4.0s
4	1.3s	0.3s (0.3s)	0.1s	0.4s	1.9s
8	1.6s	0.2s (0.2s)	0.1s	0.4s	2.2s

Table 1: Problem on microbiological and chemical reactions. Table shows CPU time for initial 10 time steps.

Kinetic adsorption and biodegradation

- Biochemical and geochemical reactions are the same as in the previous example.
- The 2D flow field for simulation biodegradation in a field-scale region $(5 \times 5m)$ and discretized with 30×30 uniformly sized elements.

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nproc	chemistry	Eulerian(assembly)	Lagrangian	grad	total
serial	11.6s	2.1s (1.9s)	2.8s	1.7s	15.3s
1	11.8s	2.1s (1.9s)	2.7s	1.7s	15.4s
2	5.8s	1.0s (0.8s)	1.3s	0.8s	7.2s
4	3.3s	0.5s (0.4s)	0.6s	0.5s	3.8s
8	2.3s	0.4s (0.3s)	0.5s	0.4s	3.0s

Table 2: Problem on kinetic adsorption and biodegradation. Table shows CPU time for initial 10 time steps.

3D Well Pumping Simulation

- 3D simulation of transport (first simulation) and transport with chemistry (second simulation).
- Steady-state flow to a pumping well.
- model boundaries are fixed head/fixed concentration, impervious, and air-soil interface (variable boundary for flow, no solute transport across top boundary)
- The flow field was calculated with 3DFEMWATER (example 3 from Yeh, 1987 ORNL-TM6386). The binary input file contains the steady-state velocity field and the moisture content data.
- First simulation: non-reactive tracer
- Second simulation: uses setup of components and species as in example ”Microbiological and chemical reactions”.

WAG 5 transport simulation

- 3D simulation of tracer experiment with steady-state flow field.
- Heterogeneous model domain (soil, matrix, fracture).
- Size of model domain is about $20 \times 40 \times 4m$.
- Mesh consists of 15376 nodes, 27000 pentahedral elements.

nproc	chemistry	Eulerian(assembly)	Lagrangian	grad	total
serial	4.9s	34.3s (26.1s)	6.1s	27.9s	74.5s
1	5.3s	34.2s (25.9s)	6.2s	27.8s	74.8s
2	1.9s	17.0s (10.5s)	2.5s	11.1s	33.6s
4	1.5s	14.7s (6.5s)	1.6s	7.2s	26.5s
8	0.7s	9.5s (3.0s)	0.8s	3.3s	15.5s

Table 5: Problem on WAG 5. Table shows time for initial 10 time steps.

nproc	chemistry	Eulerian(assembly)	Lagrangian	grad	total
serial	0.7s	2.8s (2.6s)	0.9s	3.1s	7.4s
1	0.8s	2.8s (2.6s)	0.9s	3.2s	7.6s
2	0.3s	1.3s (1.2s)	0.4s	1.4s	3.4s
4	0.3s	0.8s (0.7s)	0.3s	1.0s	2.4s
8	0.1s	0.5s (0.4s)	0.1s	0.6s	1.4s

Table 3: 3D well pumping simulation with non-reactive tracer. Table shows CPU time for initial 10 time steps.

nproc	chemistry	Eulerian(assembly)	Lagrangian	grad	total
serial	50.8s	19.3s (18.2s)	6.2s	21.4s	87.3s
1	51.5s	19.5s (18.1s)	6.2s	22.2s	88.8s
2	22.6s	8.8s (8.0s)	2.7s	10.0s	39.6s
4	13.1s	5.3s (4.7s)	1.8s	5.9s	23.7s
8	5.7s	3.3s (2.8s)	0.8s	3.4s	12.1s

Table 4: 3D well pumping simulation with reactive system. Table shows CPU time for initial 10 time steps.

Limitations (and future directions)

- Need to import hydrologic variables of flow velocity, moisture content, and pressure head generated by a subsurface flow model.
- One way effect of temperature on stability constant and kinetic rate coefficients. Assume isothermic reactions (negligible energy produced).
- Application to single-fluid phase flow (no transport of gas phase).