Parallelization of MIN3P-THCm: A high performance computational framework for subsurface flow and reactive transport simulation

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PETSc 20th Anniversary Workshop
June, 2015

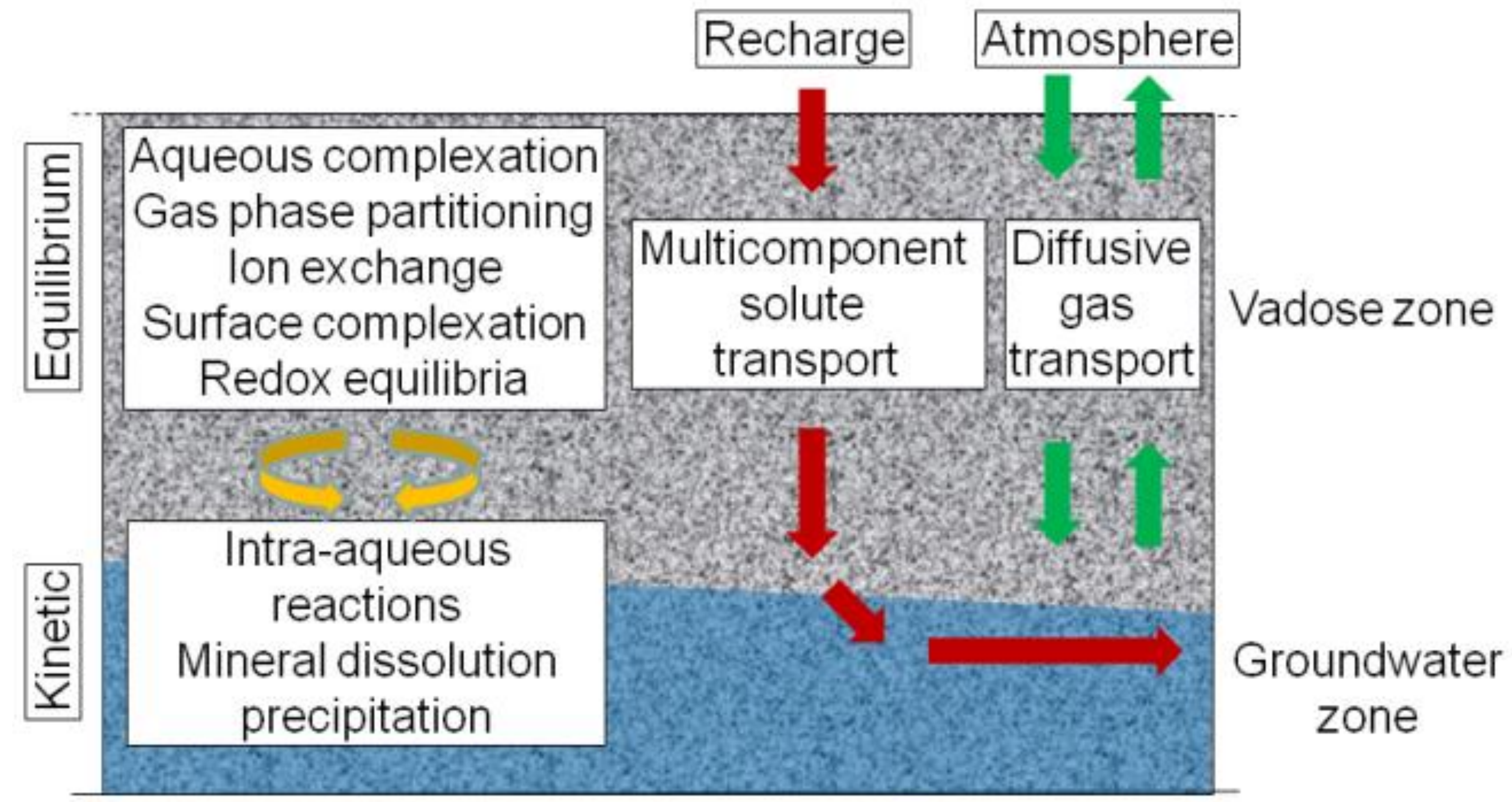
MIN3P-Basic Model (Mayer, 1998, U. Waterloo)

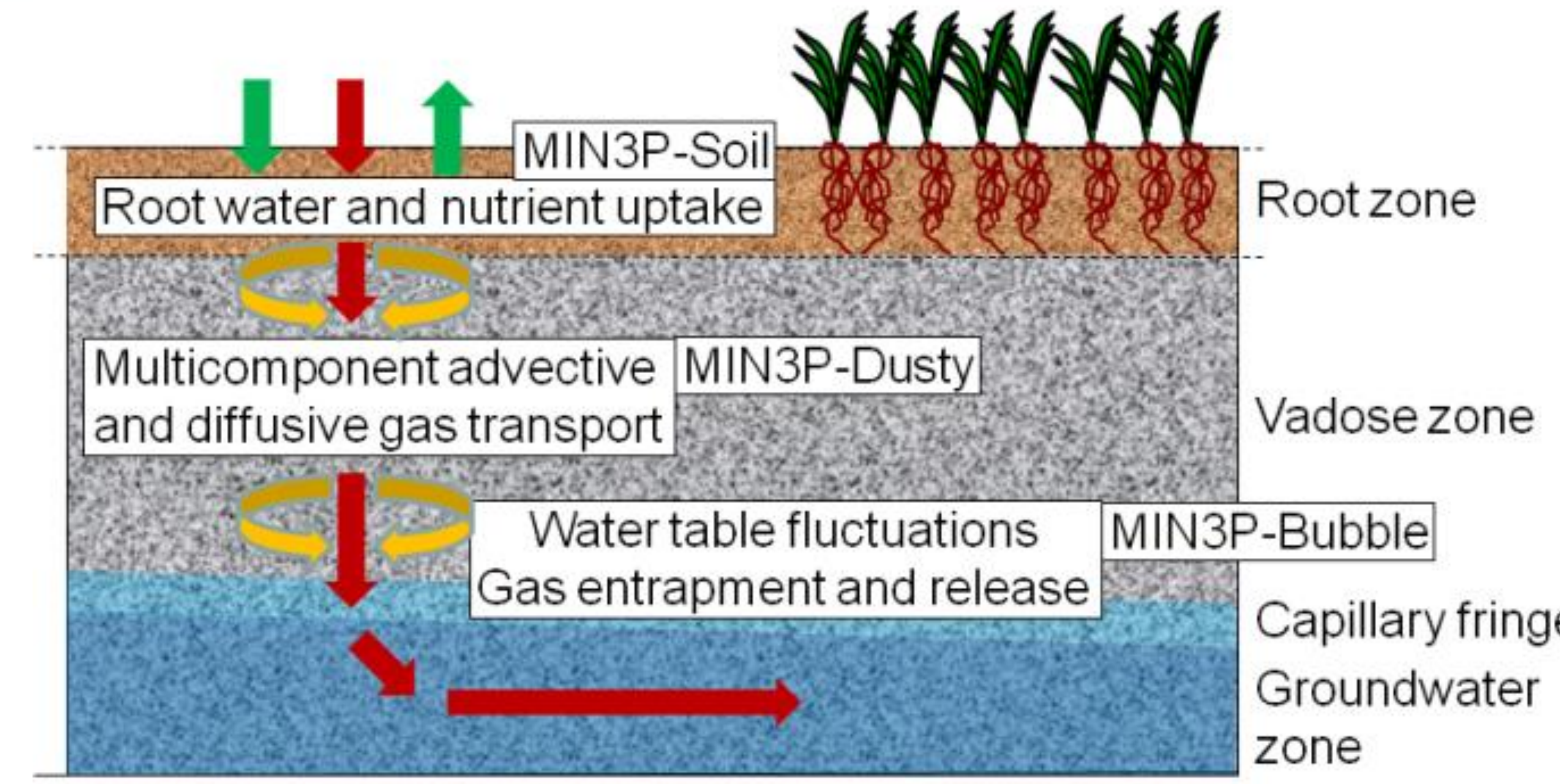
Flow

$$S_a S_s \frac{\partial h}{\partial t} + \phi \frac{\partial S_a}{\partial t} - \nabla \cdot [k_{ra} \mathbf{K} \nabla h] - Q_a = 0$$

Reactive Transport

$$\frac{\partial}{\partial t}[S_a \phi T_{ic}^a] + \frac{\partial}{\partial t}[S_g \phi T_{ic}^g] + \frac{\partial T_{ic}^s}{\partial t}$$
$$+\nabla \cdot [\mathbf{v}_a T_{ic}^a] - \nabla \cdot [S_a \phi \mathbf{D}_a \nabla T_{ic}^a] - \nabla \cdot [S_g \phi \mathbf{D}_g \nabla T_{ic}^g]$$
$$-Q_{ic}^{a,a} - Q_{ic}^{a,m} - Q_{ic}^{a,ext} - Q_{ic}^{g,ext} = 0 \qquad ic = 1, N_c$$

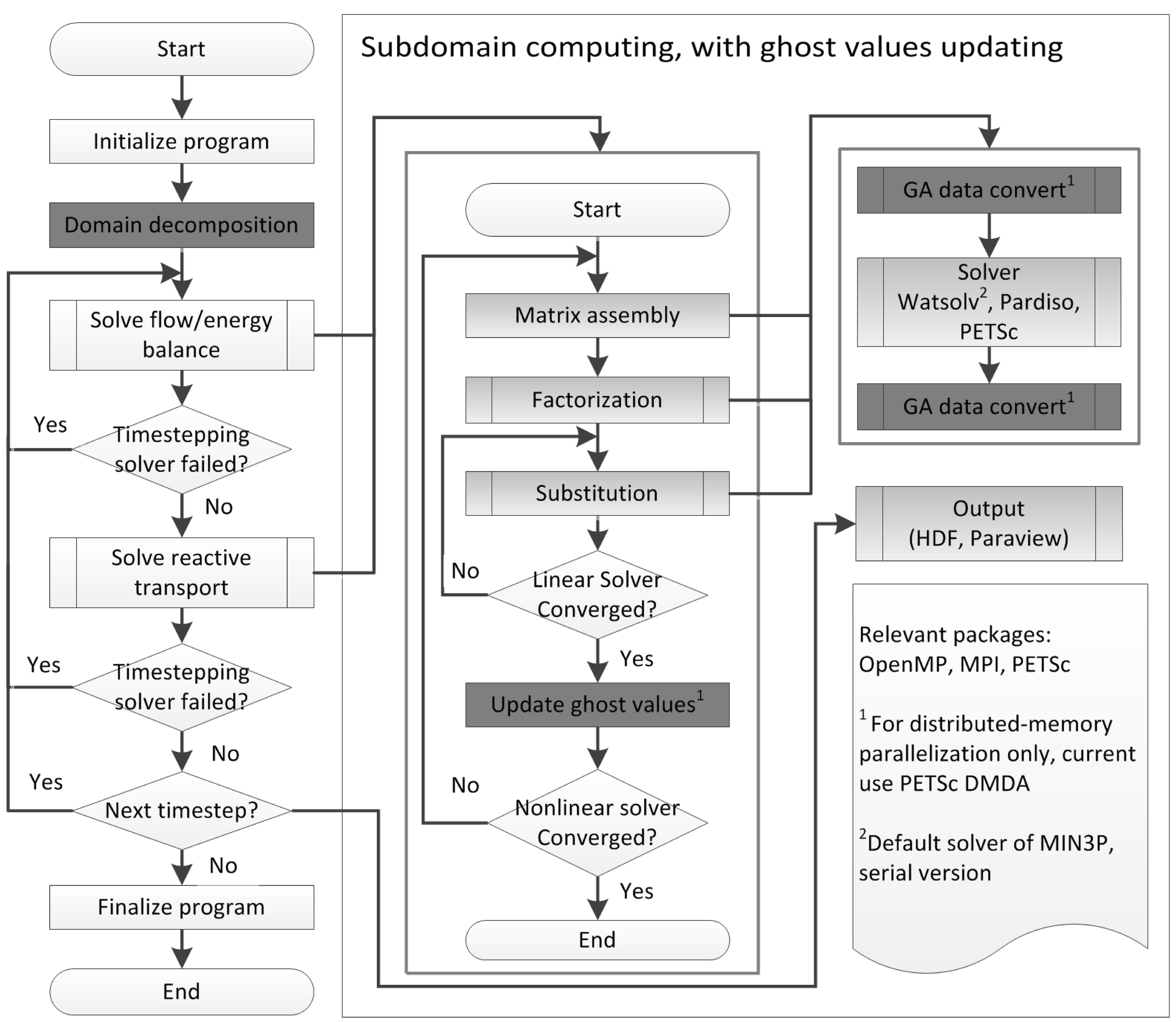




Numerical Methods: Global implicit and finite volume

Newton-Raphson linearization

ILU-preconditioned iterative solver



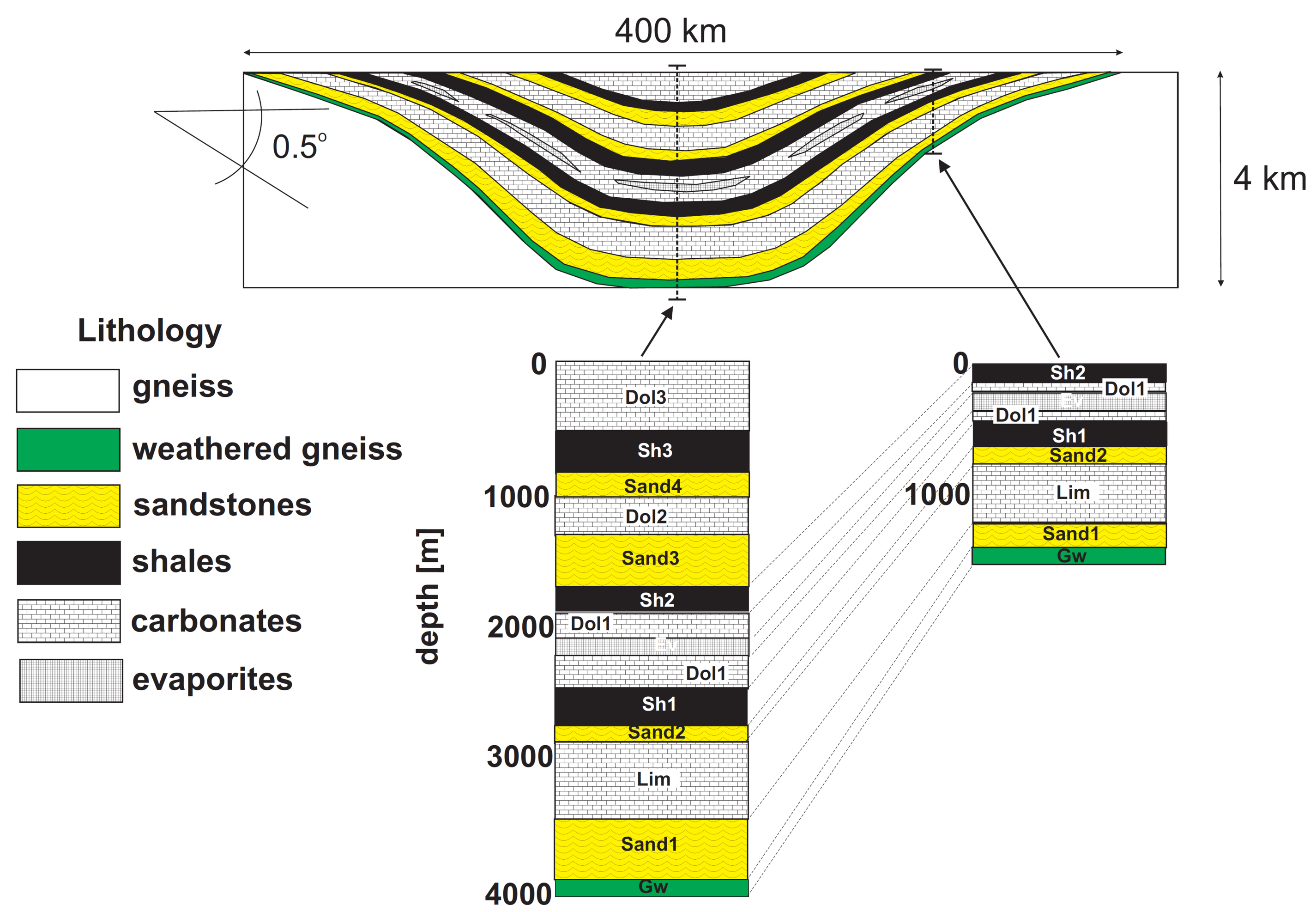
Additional development started from 2000 at UBC

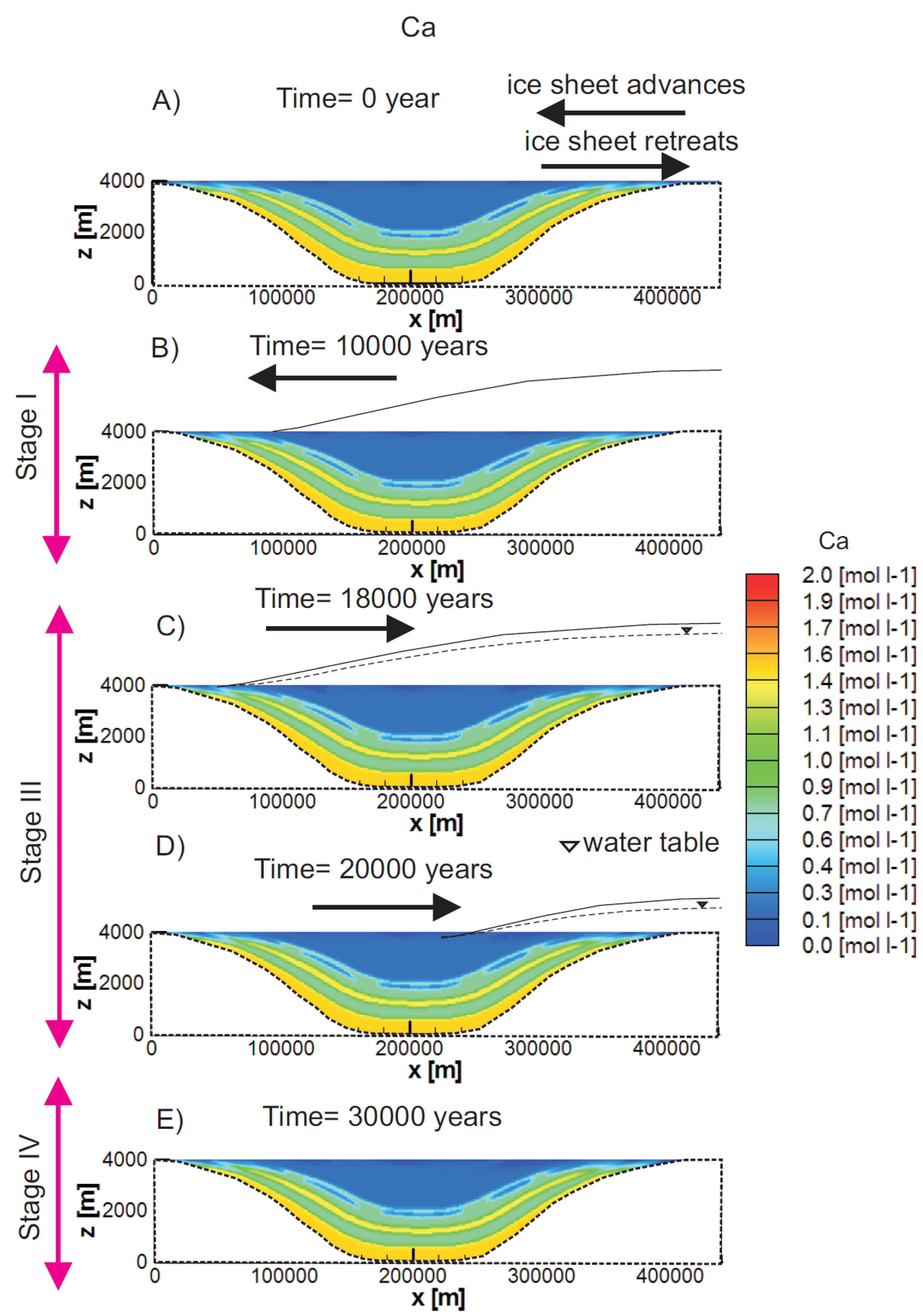
- **MIN3P-Dual (Cheng, 2006): dual porosity**
- **MIN3P-Bubble (Amos and Mayer, 2006): gas exsolution, entrapment and release**
- **MIN3P-Dusty (Molins and Mayer, 2007): gas advection and multicomponent diffusion**
- **MIN3P-Soil (Gerard, 2008): plant soil interactions**
- **MIN3P-Thcm (Bea, 2012): Pitzer equations, energy balance, vertical stress, atmospheric boundary condition**

- **MIN3P_THCm Parallelization (Su, 2015): Merge the above versions together and parallelize using OpenMP and/or MPI, PETSc**

Flow and reactive transport in a sedimentary basin

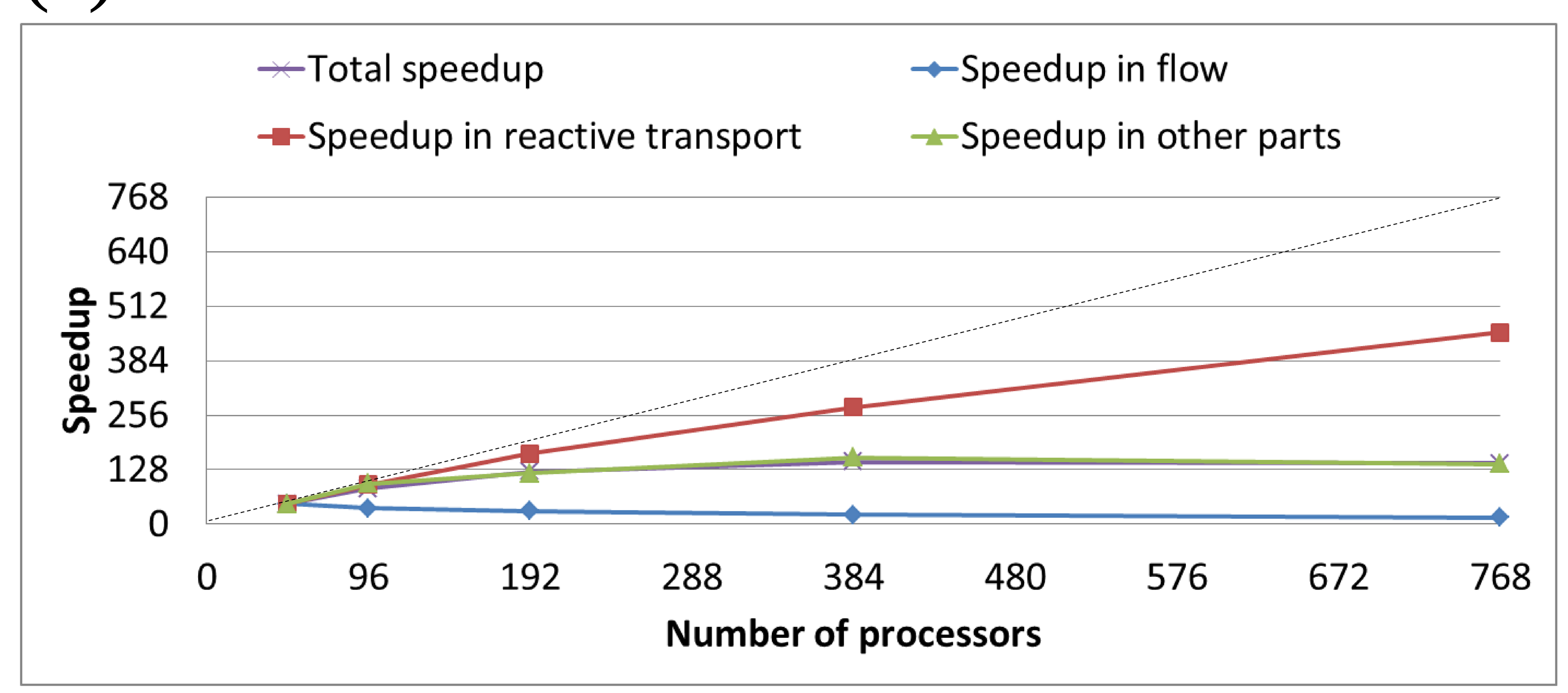
This case presents a strategy for conducting flow and reactive transport simulations in Michigan Basins affected by glaciation and deglaciation events.



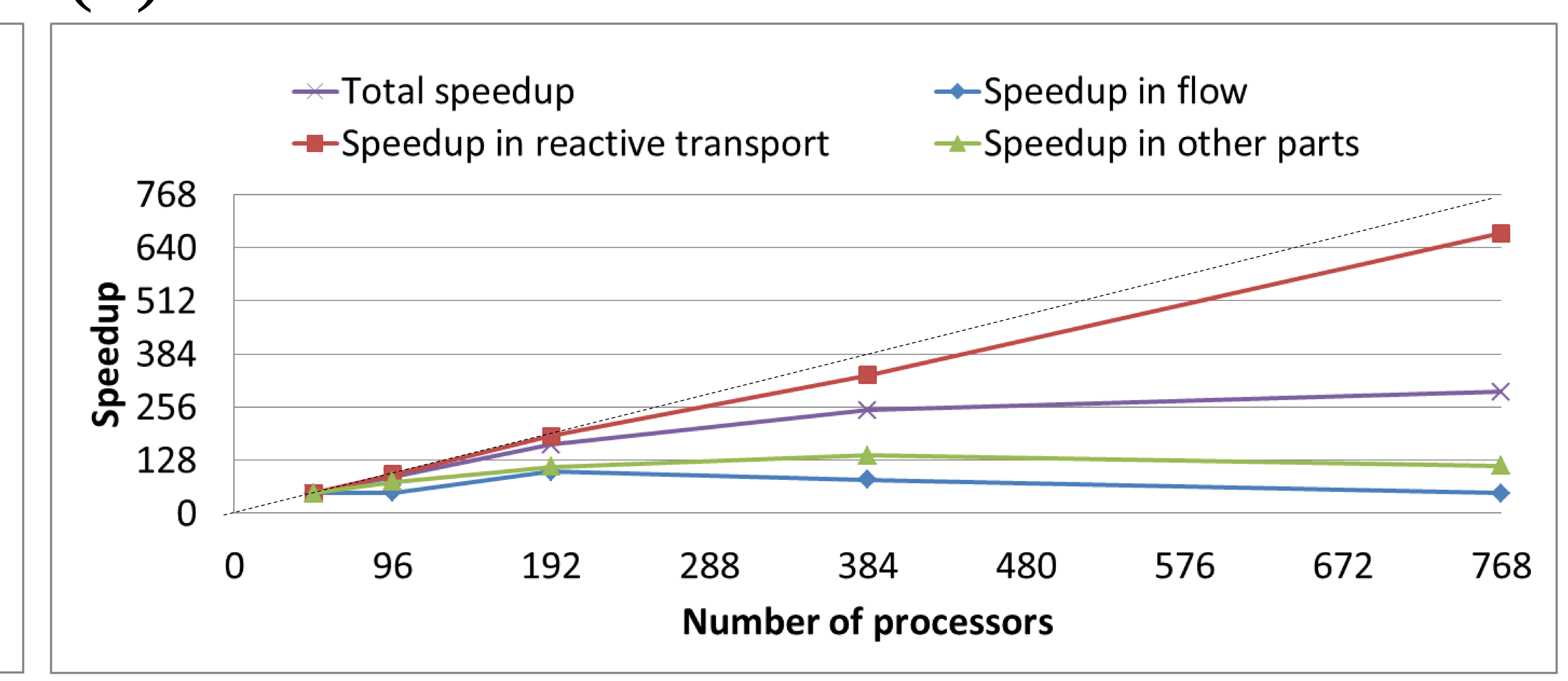


Parameters	Case (a)	Case (b)	Case (c)	Case (d)
Horizontal discretization	450	1800	3600	7200
Vertical discretization	100	400	800	1600
Total number of unknowns of flow	45000	720000	2880000	11520000
Total number of unknowns of reactive transport	405000	6480000	25920000	103680000

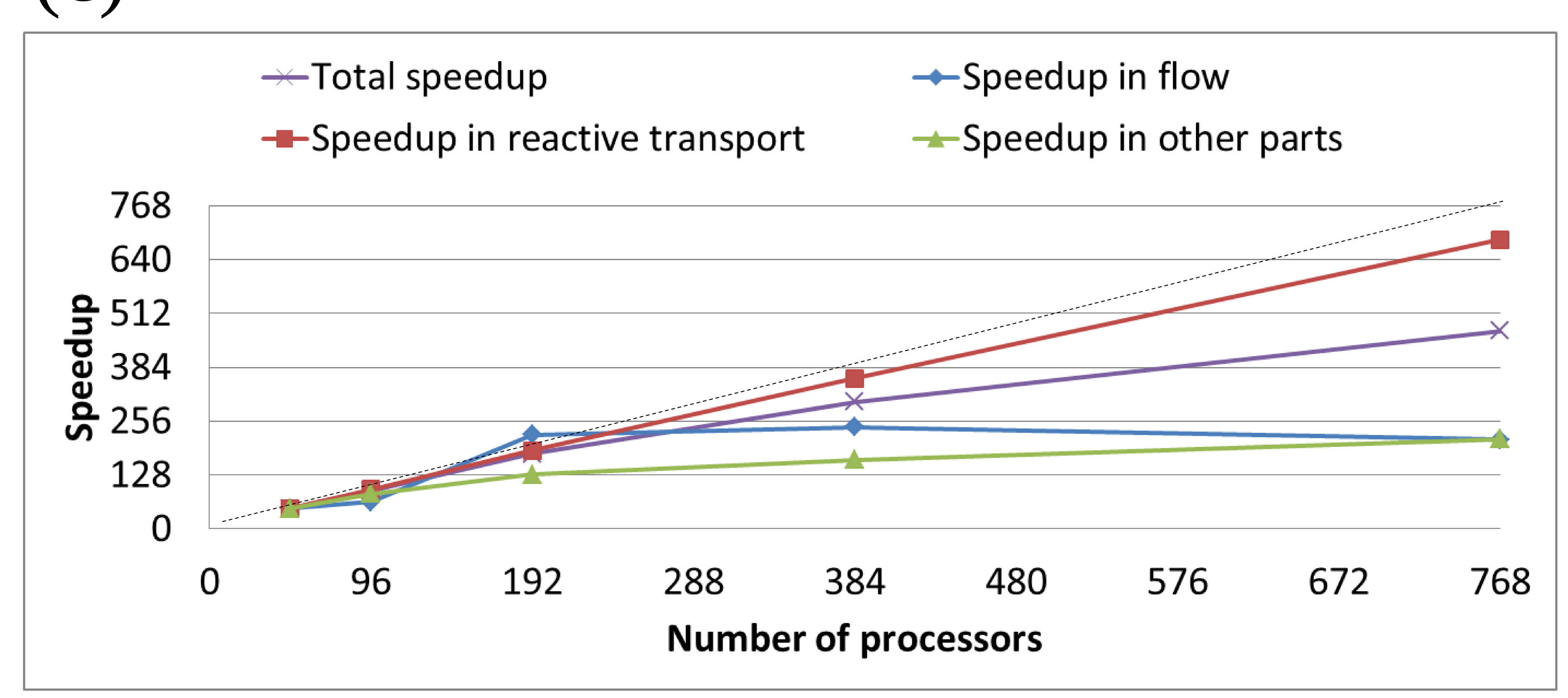
(a)



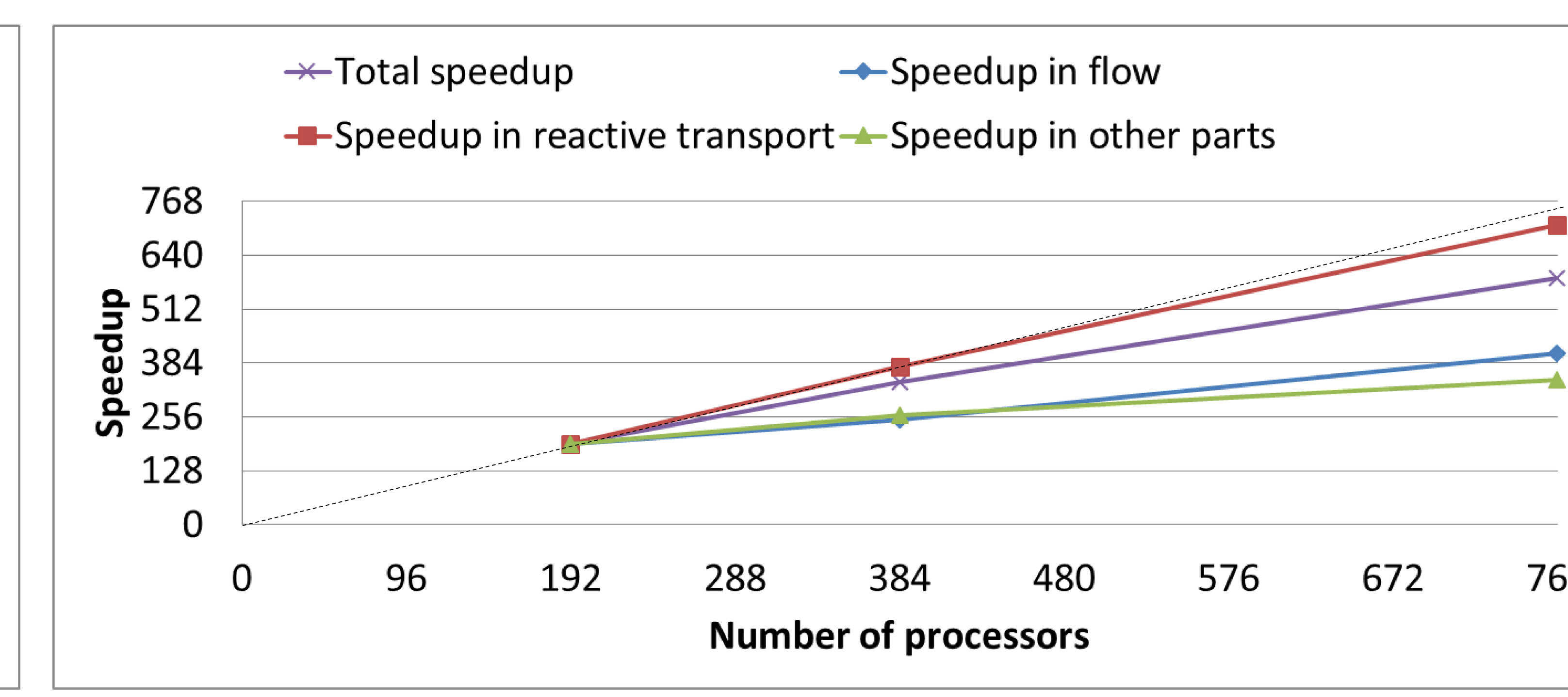
(b)



(c)



(d)



Speedup on WestGrid Jasper Cluster (Compute Canada)

The total speedup tends to be ideal when the total number of unknowns per processor > 135000.
The speedup of reactive transport part tends to be linear when the total number of unknows per processor > 33750.