Compiling and solving 100,000 equations on a PC in (3) minutes

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Outline

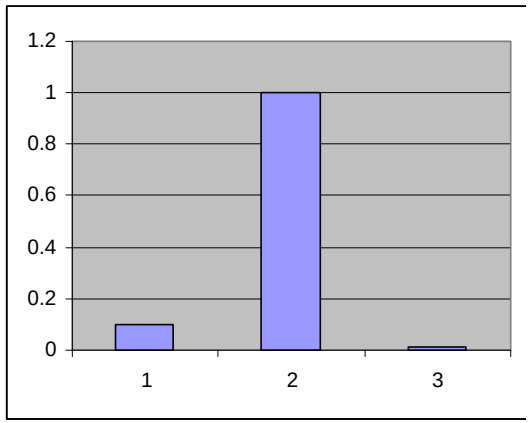
- Speeding up model solving
- Procedural vs. non-procedural modeling
- Directed acyclic graphs (DAGs)
  + Hierarchical modeling
  + Object sharing
- An DAG based algorithm to find unique equation types
- Impact on
  + compiling
  + residual and jacobian evaluation
- A DAG based algorithm to reduce L\U factorization times

Speeding up model solving

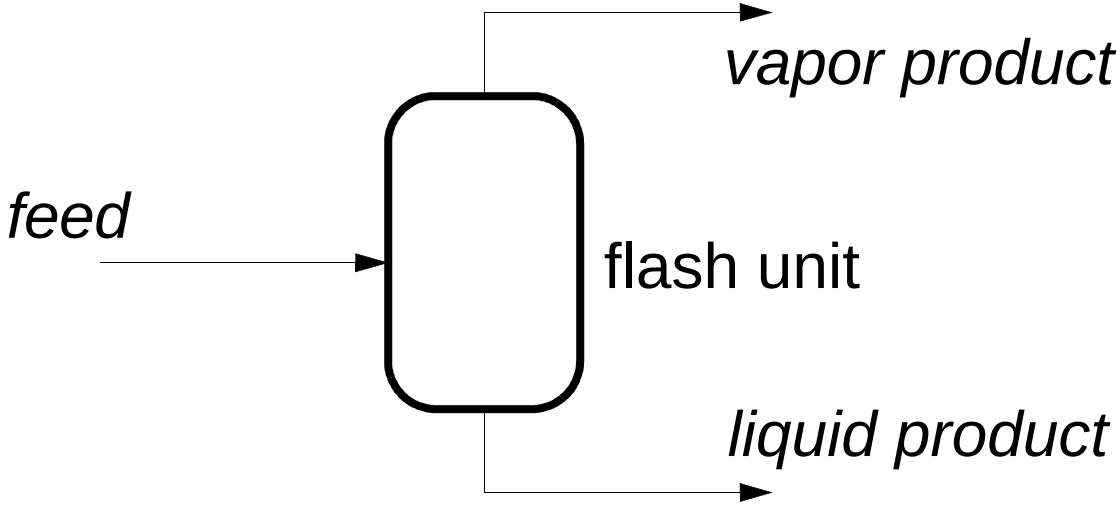
Need much faster

1.compile
2.residual and jacobian evaluation
3.L\U factorization

Failure on any one leaves a bottleneck



Equation-based vs. procedural modeling



Procedural

Given *feed* and *T, P*, write subroutine to compute *vapor* and *liquid products*

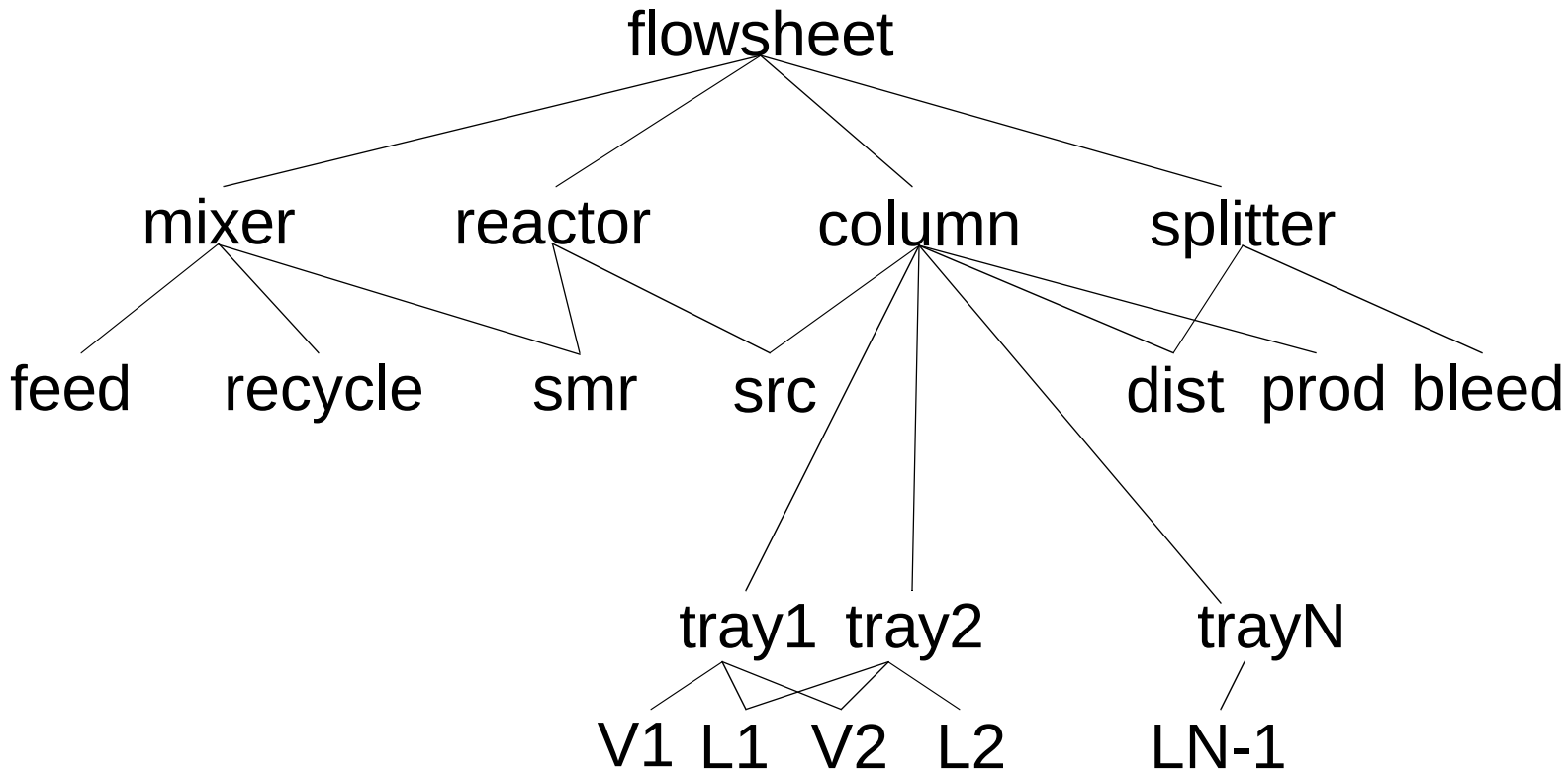
Equation-based

Fix a sufficient set of variables so model can compute the remaining *n* variables using the *n* model equations

Directed Acyclic Graphs (DAGs)

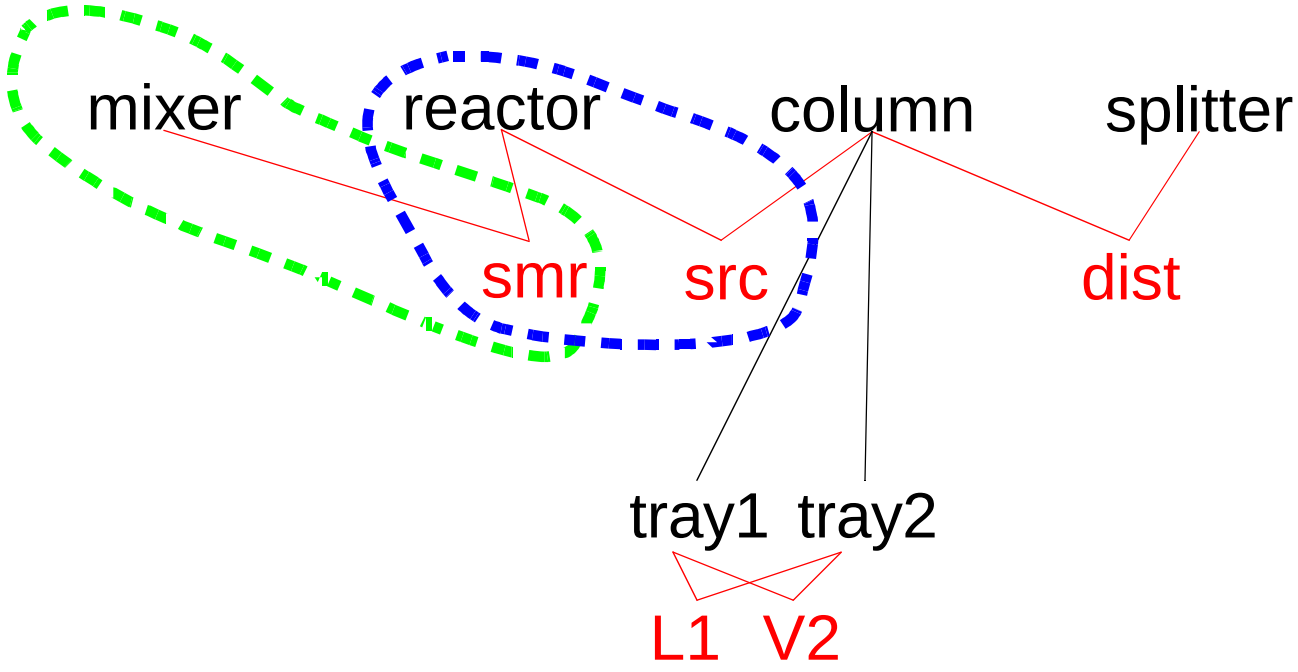
Hierarchical part/whole modeling

- to control complexity

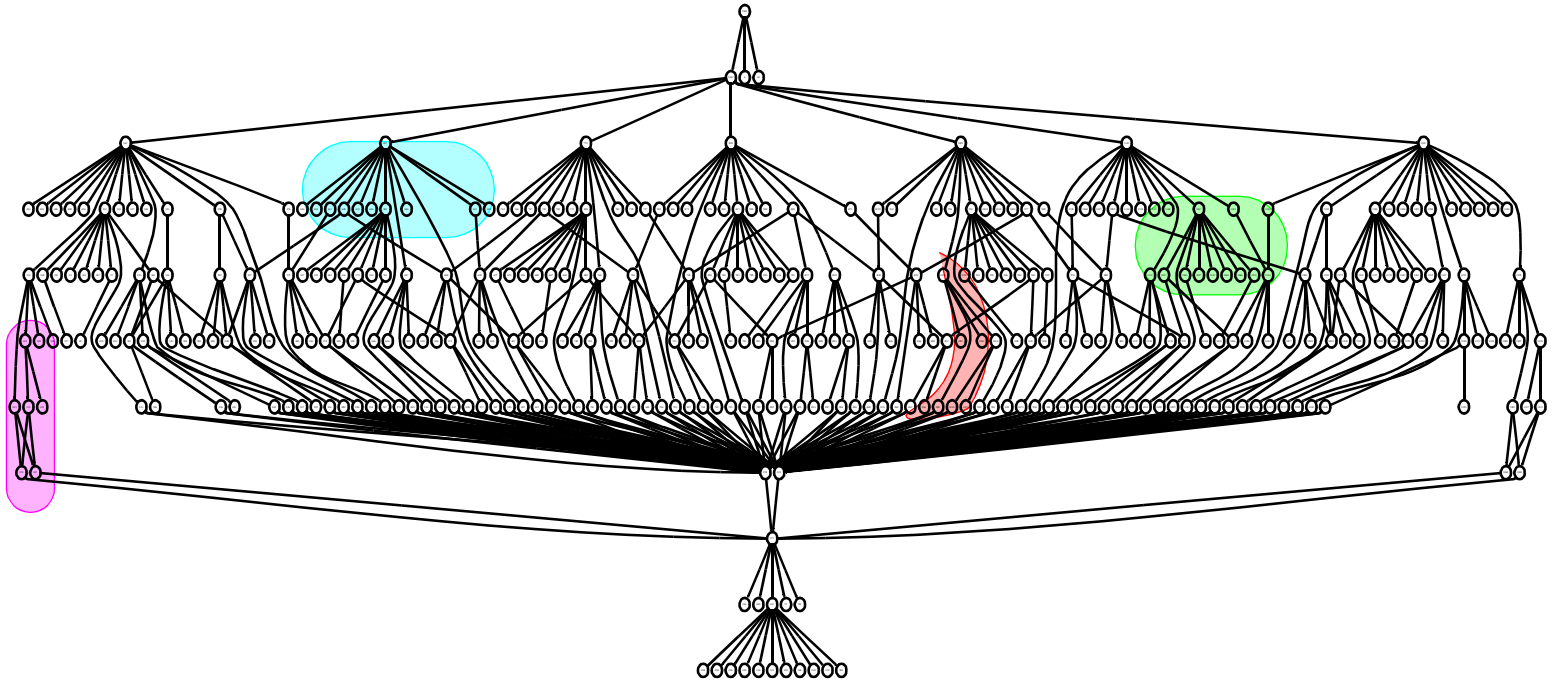


Sharing of parts to

- configure complex models in a natural way
- permit solving of isolated parts



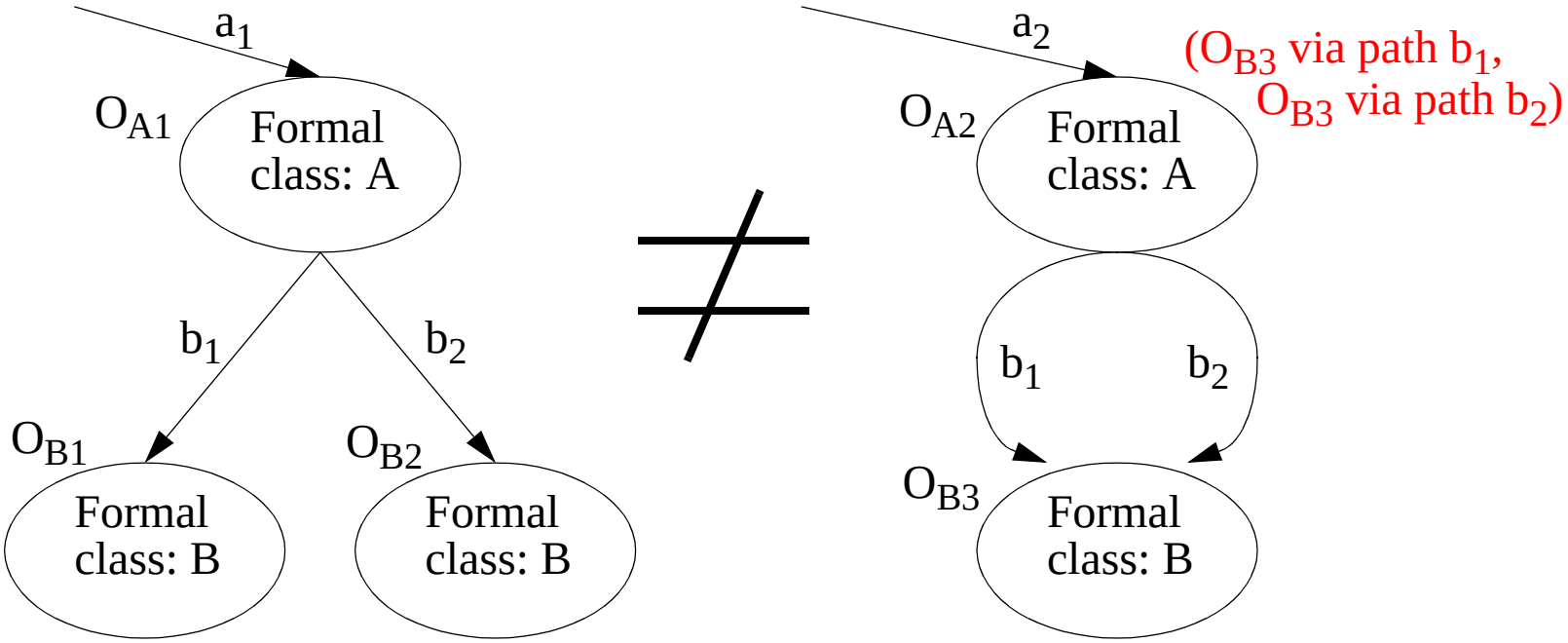
The DAG for a seven tray column



Much repeated structure

- Can we find it?
- Can we then use that information?

Anonymous types

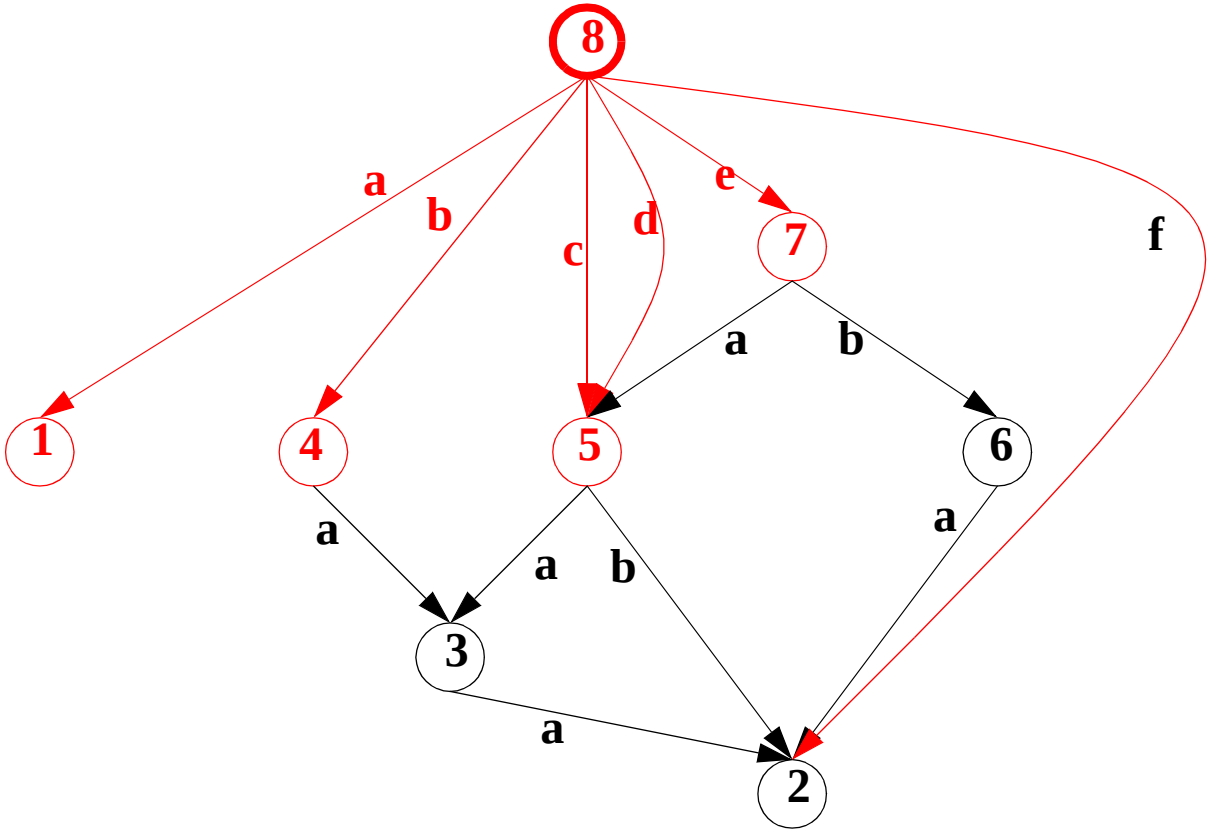


Algorithm

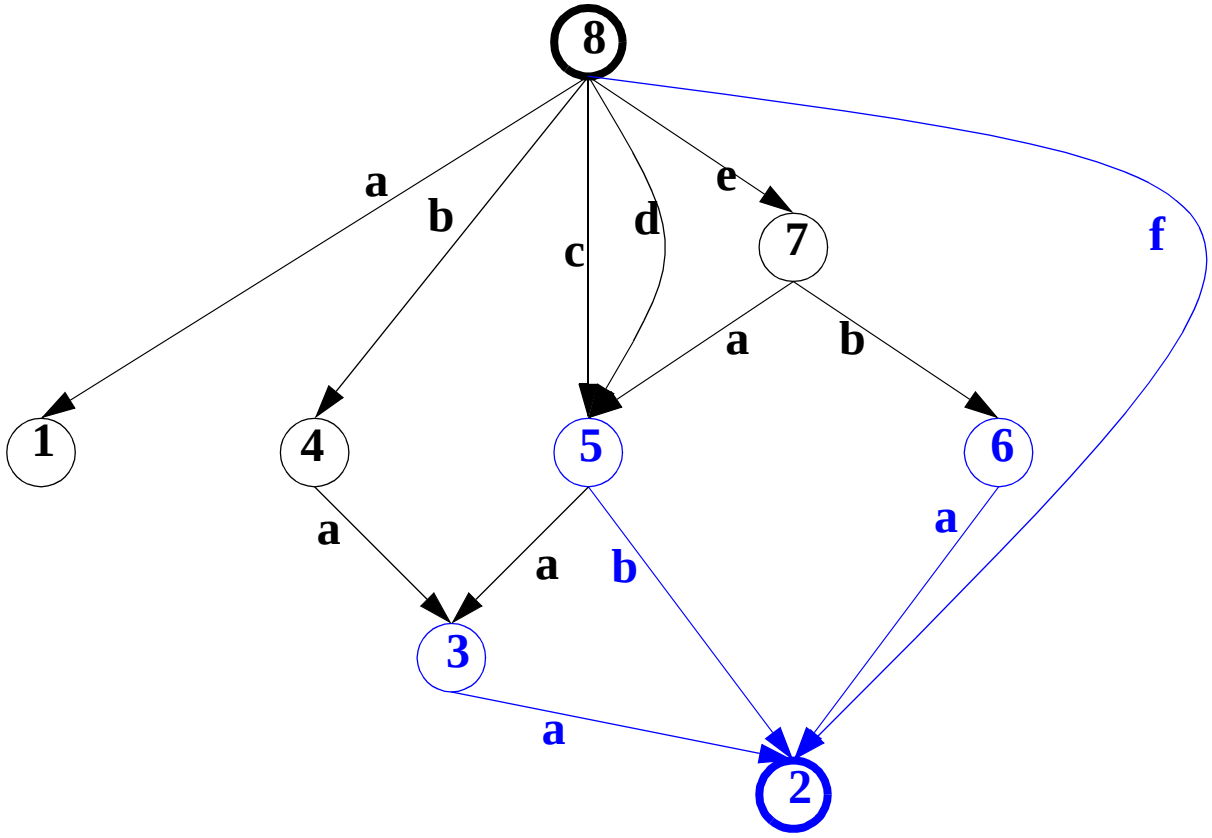
- For all nodes *i*
  + Construct list of visible nodes
- For all node pairs *i* and *j*
  + Find all independent paths *i* to *j*
  + Label node *i* with such paths

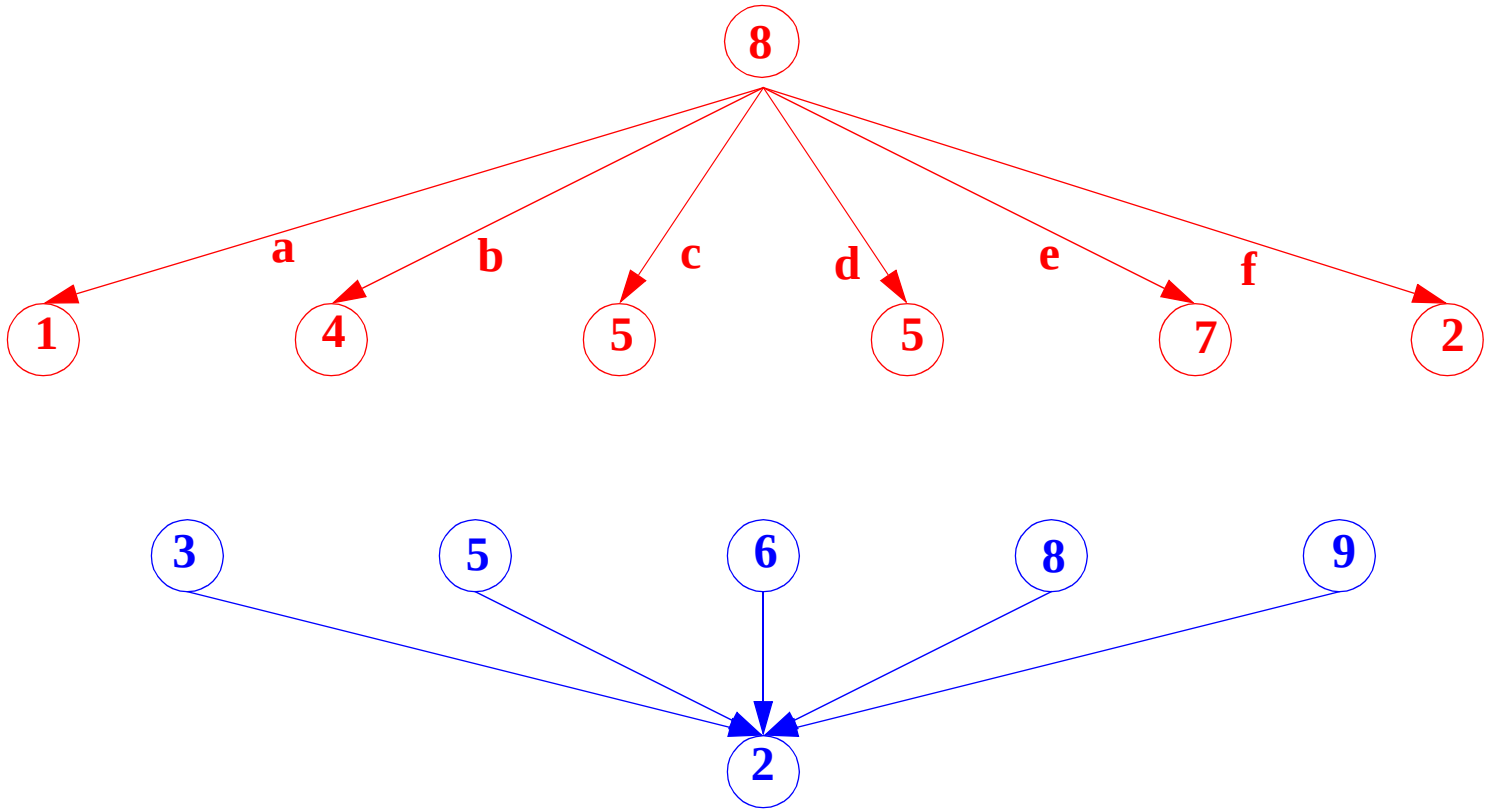
Provably order n^4; experience linear growth

Children of node *i* (8)

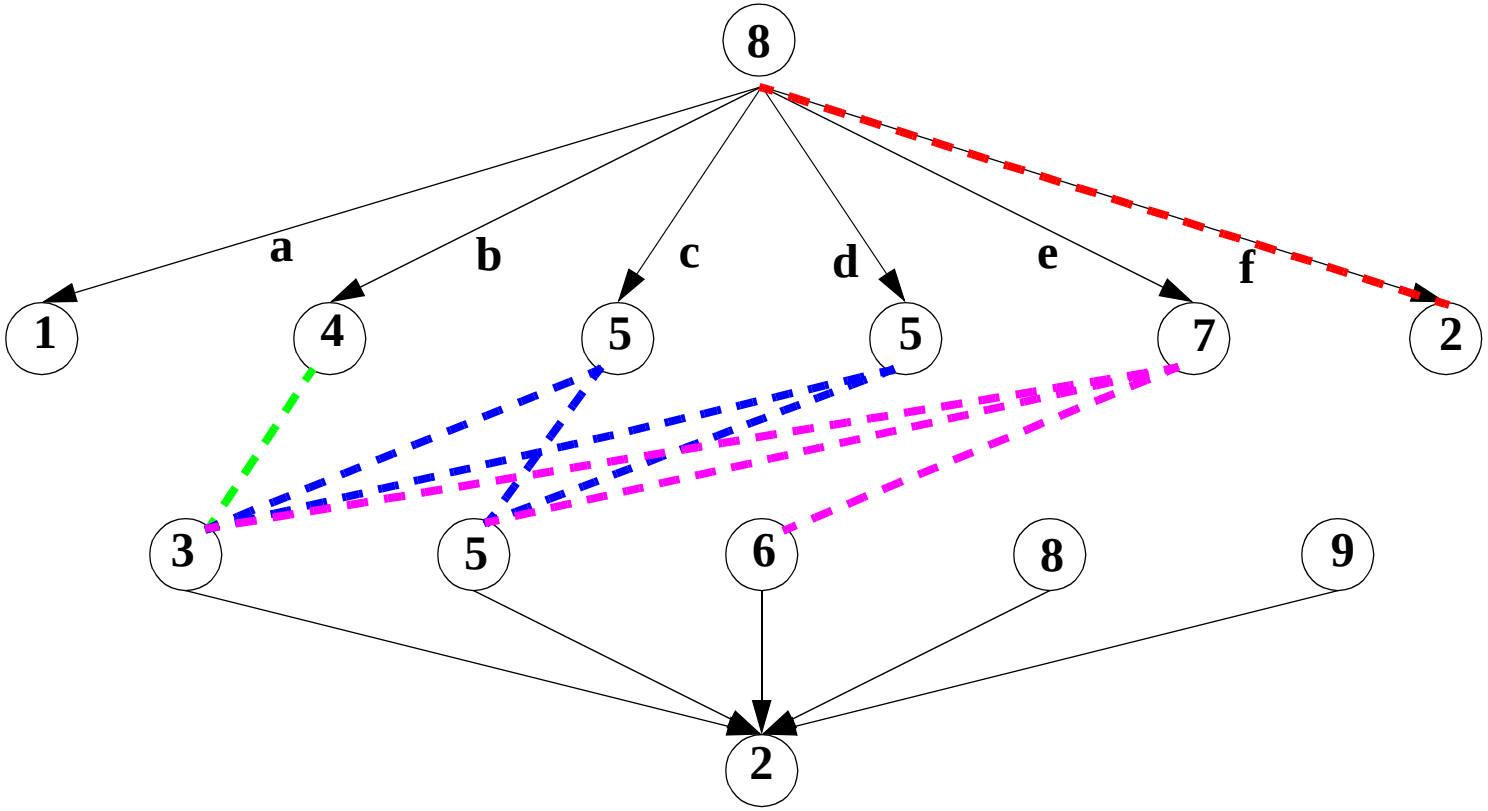


Parents of node *j* (2)

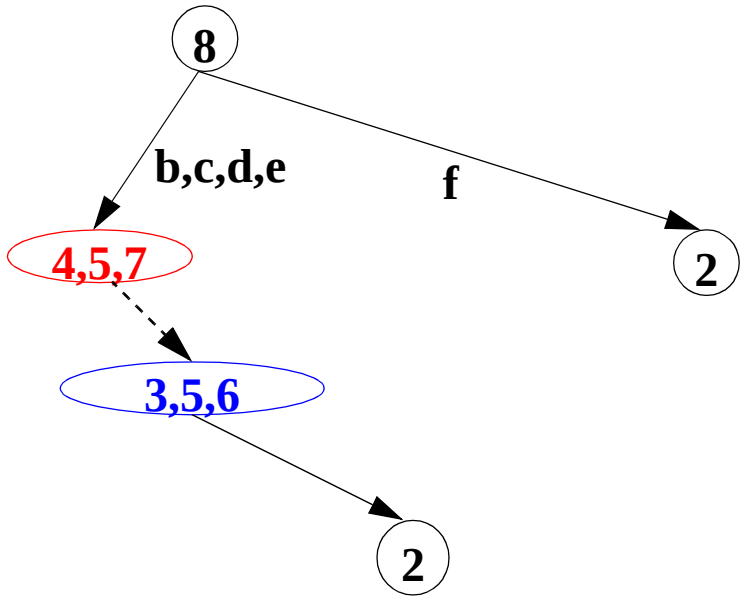



8
a
b
c
d
e
f
1
4
5
5
7
2
3
5
6
8
9
2

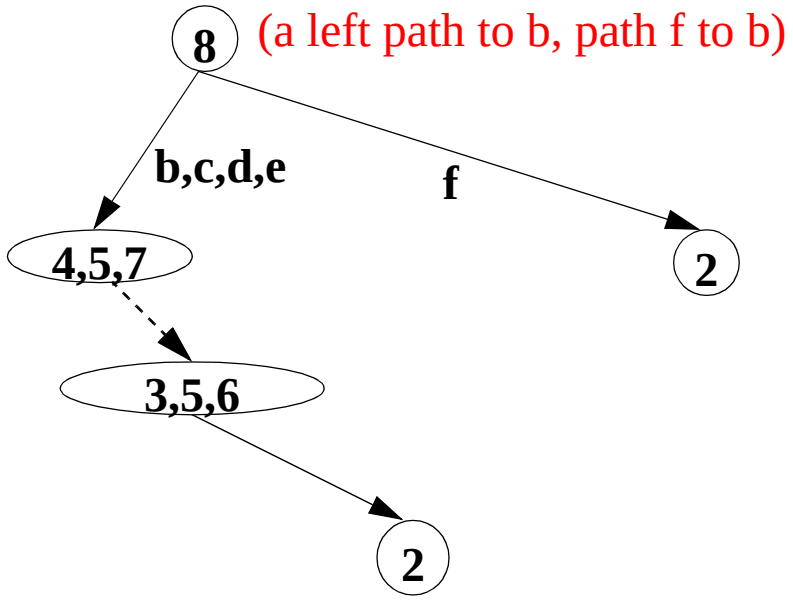
Parents of *j* seen by children of *i*



Collapse graph; spot independent paths



Label node *i*



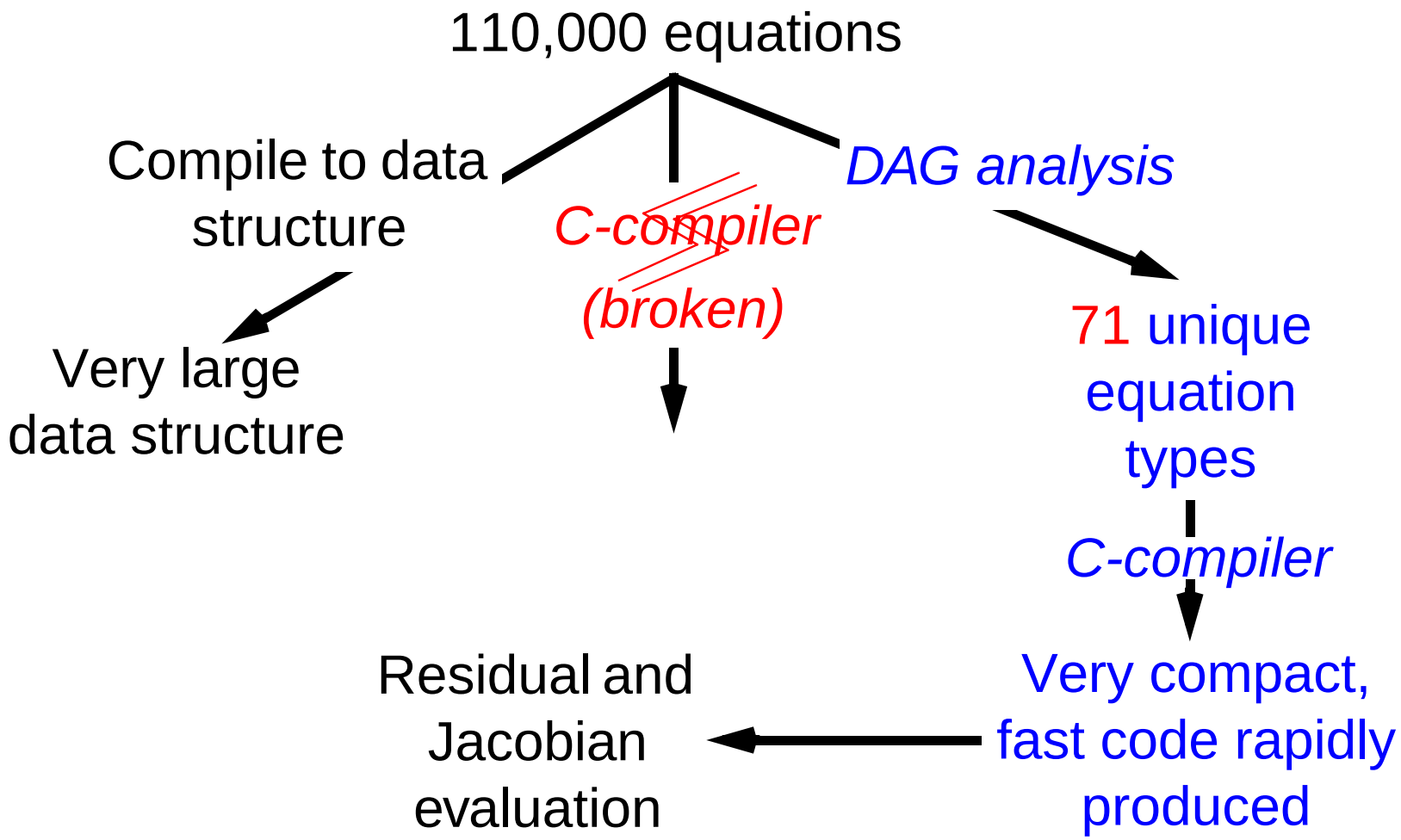
Very fast compile

We now compile at the rate of
120,000 equations/minute on
200 megahertz pentium PC

and solve

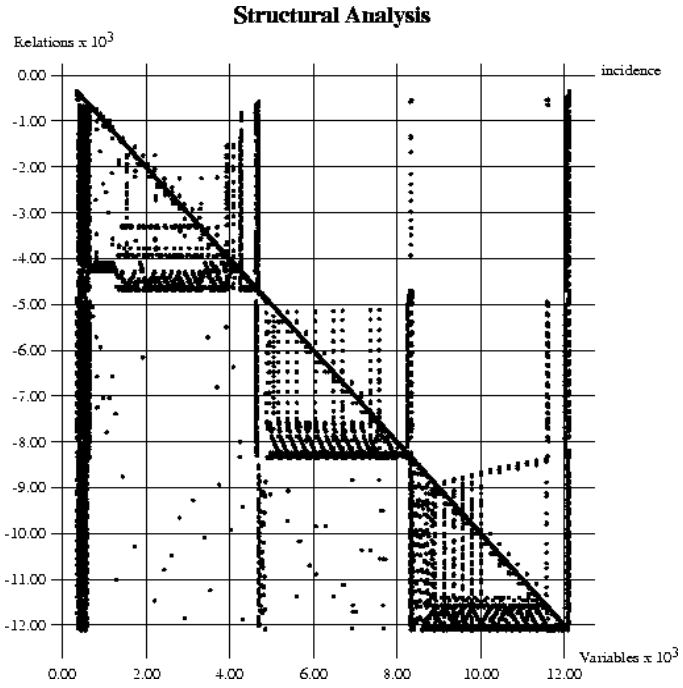
Residual evaluation is at
230,000 equations/second on
200 megahertz pentium PC

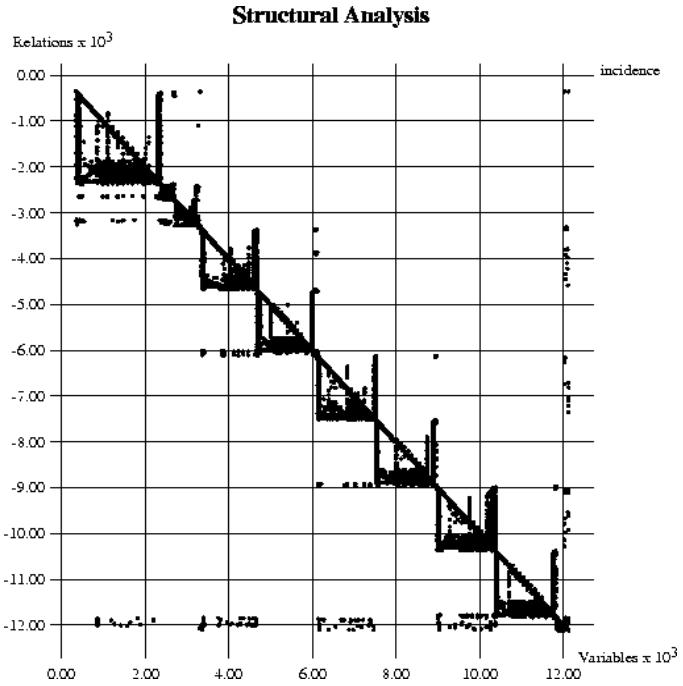
Why so fast?

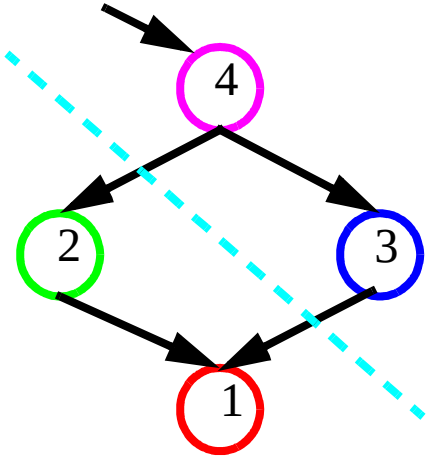

110,000 equations
Compile to data structure
C-compiler
(broken)
DAG analysis
Very large data structure
71 unique equation types
C-compiler
Very compact, fast code rapidly produced
Residual and Jacobian evaluation

Reducing fill for L\U factorization

- DAG-based algorithm pre-orders equations
- Recursive bisection at object boundaries







	1	2	3	4	***5***	6	7	8
1	***X***	x		x				
2	***x***	**X**	x					
3			**X**	x				
4				**X**	***x***			
5						**X**	x	x
6						x	**X**	
7	***x***						x	**X**
8					***X***		x	

L\U factorization speeds

Times reduced by factors of 5 to 10

Ex:

83,000 equations (53,000 equation partition) preordered in 15.5 sec and factored in 4 sec on 150 megahertz UNIX workstation

In conclusion

DAG-based algorithms to speed up

- compiling
- evaluating residuals and jacobians
- finding BBD structure for L\U factoring

to meet the goal to

Compile and solve 100,000 equations (flow-sheet modeling) in three minutes on a PC