CHW Example 6.5

Loads the chemJac command file, which contains all commands used below

```
(*  SetDirectory["C:\CHEMmma"] *) (* Put in path to chemJac.m *)
<< "chemJac.m"
```

```
C:\CHEMmma
```

```
chemJac is loading...
```

```
chemJac has loaded
```

Inputting the stoichiometric matrix S (we input half the matrix and then use the "makeReversible" command)

```
S = Transpose[{{-1, -1, 0, 0, 1, 0, 0},
    {0, -1, -1, 0, 0, 1, 0}, {0, 0, -1, -1, 0, 0, 1}, {2, 0, 0, -1, 0, 0, 0}}];
S = makeReversible[S];
S // MatrixForm
```

$$\begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 & 2 & -2 \\ -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 & -1 & 1 \\ 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \end{pmatrix}$$

Making the non-mass-action flux vector 'monomials' and the list of species concentrations 'vars' automatically from S

```
monomials = makeMonomialNMA[S]
```

```
{k[1][a[1], a[2]], k[2][a[5]], k[3][a[2], a[3]],
 k[4][a[6]], k[5][a[3], a[4]], k[6][a[7]], k[7][a[4]], k[8][a[1]]}
```

```
vars = svars[S]
```

```
{a[1], a[2], a[3], a[4], a[5], a[6], a[7]}
```

'S.monomials' is the right hand side of the ODE

```
S.monomials
```

```
{-k[1][a[1], a[2]] + k[2][a[5]] + 2 k[7][a[4]] - 2 k[8][a[1]],
 -k[1][a[1], a[2]] + k[2][a[5]] - k[3][a[2], a[3]] + k[4][a[6]],
 -k[3][a[2], a[3]] + k[4][a[6]] - k[5][a[3], a[4]] + k[6][a[7]],
 -k[5][a[3], a[4]] + k[6][a[7]] - k[7][a[4]] + k[8][a[1]], k[1][a[1], a[2]] - k[2][a[5]],
 k[3][a[2], a[3]] - k[4][a[6]], k[5][a[3], a[4]] - k[6][a[7]]}
```

The Jacobian of the RHS of the ODE, and its Craciun-Feinberg determinant

```
j = jac[S.monomials, vars];
j // MatrixForm
```

$$\begin{pmatrix} -2\,k[8]'[a[1]] - k[1]^{(1,0)}[a[1], a[2]] & -k[1]^{(0,1)}[a[1], a[2]] & \\ -k[1]^{(1,0)}[a[1], a[2]] & -k[1]^{(0,1)}[a[1], a[2]] - k[3]^{(1,0)}[a[2], a[3]] & -k[\\ 0 & -k[3]^{(1,0)}[a[2], a[3]] & -k[3]^{(0,1)}[a[2] \\ k[8]'[a[1]] & 0 & -k[\\ k[1]^{(1,0)}[a[1], a[2]] & k[1]^{(0,1)}[a[1], a[2]] & \\ 0 & k[3]^{(1,0)}[a[2], a[3]] & k[\\ 0 & 0 & k[\end{pmatrix}$$

```
det = cfDet[j]; (* output not shown due to length! *)

coeffs[det]
```

The number of terms in the det expansion is 138,

and (a,b) says that the number of terms with coef a is b:

```
{{-3, 2}, {-2, 40}, {-1, 96}}
```

Core Determinant of the Jacobian of the RHS of the ODE

```
core = coreDet[j, S]
```

```
-k[2]'[a[5]] k[4]'[a[6]] k[6]'[a[7]] k[7]'[a[4]] - 2 k[2]'[a[5]] k[4]'[a[6]] k[6]'[a[7]] k[8]'[a[1]] -
 k[4]'[a[6]] k[6]'[a[7]] k[7]'[a[4]] k[1]^(0,1)[a[1], a[2]] -
 2 k[4]'[a[6]] k[6]'[a[7]] k[8]'[a[1]] k[1]^(0,1)[a[1], a[2]] -
 k[2]'[a[5]] k[6]'[a[7]] k[7]'[a[4]] k[3]^(0,1)[a[2], a[3]] -
 2 k[2]'[a[5]] k[6]'[a[7]] k[8]'[a[1]] k[3]^(0,1)[a[2], a[3]] -
 k[6]'[a[7]] k[7]'[a[4]] k[1]^(0,1)[a[1], a[2]] k[3]^(0,1)[a[2], a[3]] -
 2 k[6]'[a[7]] k[8]'[a[1]] k[1]^(0,1)[a[1], a[2]] k[3]^(0,1)[a[2], a[3]] -
 2 k[2]'[a[5]] k[4]'[a[6]] k[8]'[a[1]] k[5]^(0,1)[a[3], a[4]] -
 2 k[4]'[a[6]] k[8]'[a[1]] k[1]^(0,1)[a[1], a[2]] k[5]^(0,1)[a[3], a[4]] -
 2 k[2]'[a[5]] k[8]'[a[1]] k[3]^(0,1)[a[2], a[3]] k[5]^(0,1)[a[3], a[4]] -
 3 k[8]'[a[1]] k[1]^(0,1)[a[1], a[2]] k[3]^(0,1)[a[2], a[3]] k[5]^(0,1)[a[3], a[4]] -
 k[4]'[a[6]] k[6]'[a[7]] k[7]'[a[4]] k[1]^(1,0)[a[1], a[2]] -
 k[6]'[a[7]] k[7]'[a[4]] k[3]^(0,1)[a[2], a[3]] k[1]^(1,0)[a[1], a[2]] -
 k[2]'[a[5]] k[6]'[a[7]] k[7]'[a[4]] k[3]^(1,0)[a[2], a[3]] -
 2 k[2]'[a[5]] k[6]'[a[7]] k[8]'[a[1]] k[3]^(1,0)[a[2], a[3]] -
 2 k[2]'[a[5]] k[8]'[a[1]] k[5]^(0,1)[a[3], a[4]] k[3]^(1,0)[a[2], a[3]] -
 k[6]'[a[7]] k[7]'[a[4]] k[1]^(1,0)[a[1], a[2]] k[3]^(1,0)[a[2], a[3]] -
 k[2]'[a[5]] k[4]'[a[6]] k[7]'[a[4]] k[5]^(1,0)[a[3], a[4]] -
 2 k[2]'[a[5]] k[4]'[a[6]] k[8]'[a[1]] k[5]^(1,0)[a[3], a[4]] -
 k[4]'[a[6]] k[7]'[a[4]] k[1]^(0,1)[a[1], a[2]] k[5]^(1,0)[a[3], a[4]] -
 2 k[4]'[a[6]] k[8]'[a[1]] k[1]^(0,1)[a[1], a[2]] k[5]^(1,0)[a[3], a[4]] -
 k[4]'[a[6]] k[7]'[a[4]] k[1]^(1,0)[a[1], a[2]] k[5]^(1,0)[a[3], a[4]] -
 k[2]'[a[5]] k[7]'[a[4]] k[3]^(1,0)[a[2], a[3]] k[5]^(1,0)[a[3], a[4]] -
 2 k[2]'[a[5]] k[8]'[a[1]] k[3]^(1,0)[a[2], a[3]] k[5]^(1,0)[a[3], a[4]] -
 3 k[7]'[a[4]] k[1]^(1,0)[a[1], a[2]] k[3]^(1,0)[a[2], a[3]] k[5]^(1,0)[a[3], a[4]]
```

coeffs[**core**]

The number of terms in the det expansion is 26,

and (a,b) says that the number of terms with coef a is b:

{{−3, 2}, {−2, 12}, {−1, 12}}