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Science Day

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FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

Previously

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- Nottingham Physiology Simulator:
  - Obtained as a Matlab Script.
  - Calls several functions, including 2 C-code files (pre-loaded as MEX).
- Simulator needs to be parallelised:
  - Konstantin -> RWTH Cluster
  - Chadi -> JSC Cluster
- JSC Cluster has no working Matlab implementation:
  - Octave is too complicated to set up and too many hurdles.
  - Convert the Simulation to C and run on cluster.
- Exported the simulation in C and produced initial outputs.

New Hurdles

- Further testing showed difference in outputs either immediately or after some cycles.
- Some simulations take much longer than expected.
- Diving deeper into the code difficult due to lack of documentation.
- Simulation on Matlab shows same signs as exported C-code.
- Simulation runs normally when calling MEX functions.

- Problem must be in the converted code (from C to Matlab):
  - Some of the functions were already available in the original simulation and were copied.
  - Others had to be rewritten, but C to Matlab is straightforward.
- Issue persisted.

Lightbulb Moment

- The C code is written around the proprietary mex.h library.
- Communication between this code and Matlab is in both directions.
- Aside from the variables *clearly* denoted as outputs, the function also updates (and saves) parameters that were in the inputs.
- Specifically:
  - Compartment Pressure.
  - Compartment gas volumes.

```
void mexFunction(int nlhs, mxArray* plhs[], int nrhs, const mxArray* prhs[]) {

    double  tempH2O, t4, ScapO2, Pb, SVPh2o, movedGas, nPtoS, k1, pk, k2, fBE, Temperature, pH_acc, vfrc, ColVol, *P_ext, *ST_alv;
    double  CcapO2, CcapCO2, CcapN2, CcapGas5, PccapO2, PccapCO2, Ncomp,
            PccapN2, PccapGas5, pHc, HCO3c, VcapN2, VcapGas5, VcapCO2, VcapO2;
    double  SvO2, CvO2, CvCO2, CvN2, CvGas5, PvO2, PvCO2, PvN2, PvGas5, pHv, HCO3v;
    double  *input1, *Vcomp, *Qcomp, *Pcomp, *VcompO2, *VcompCO2, *VcompN2, *VcompGas5, *VcompH2O,
            *outO2c, *outCO2c, *outN2c, *outGas5c,
            *outPalvO2, *outPccapO2;
    bool  DoneEquilib, loopcounter;
    int compN, loop2, i;
    double TotGas, t1, t2, t3, EquilAcc, Hufner, Hb, O2sol, O2solT, tempO2, Gas5PC;

    double   PalvO2, PalvCO2, PalvN2, PalvGas5, PalvH2O, outofVtoP;

    Pb =*(mxGetPr(mexGetVariablePtr("caller", "Pb")));
    SVPh2o = *(mxGetPr(mexGetVariablePtr("caller", "SVPh2o")));
    Hufner = *(mxGetPr(mexGetVariablePtr("caller", "Hufner")));
    Hb = *(mxGetPr(mexGetVariablePtr("caller", "Hb")));
    O2sol = *(mxGetPr(mexGetVariablePtr("caller", "O2sol")));
    O2solT =*(mxGetPr(mexGetVariablePtr("caller", "O2solT")));
    EquilAcc =*(mxGetPr(mexGetVariablePtr("caller", "EquilAcc")));
    Gas5PC = *(mxGetPr(mexGetVariablePtr("caller", "Gas5PC")));
    fBE =*(mxGetPr(mexGetVariablePtr("caller", "BEa")));
    Temperature =*(mxGetPr(mexGetVariablePtr("caller", "Temperature")));
    pH_acc =*(mxGetPr(mexGetVariablePtr("caller", "pH_acc")));
    vfrc= *(mxGetPr(mexGetVariablePtr("caller", "Vfrc")));
    Ncomp =*(mxGetPr(mexGetVariablePtr("caller", "Ncomp")));
    ColVol= *(mxGetPr(mexGetVariablePtr("caller", "ColVol")));
    P_ext= (mxGetPr(mexGetVariablePtr("caller", "P_ext")));
    ST_alv= (mxGetPr(mexGetVariablePtr("caller", "ST_alv")));

    input1=mxGetPr(prhs[0]);
    Vcomp=mxGetPr(prhs[1]);
    Qcomp=mxGetPr(prhs[2]);
    Pcomp=mxGetPr(prhs[3]);
    VcompO2=mxGetPr(prhs[4]);
    VcompCO2=mxGetPr(prhs[5]);
    VcompN2=mxGetPr(prhs[6]);
    VcompGas5=mxGetPr(prhs[7]);
    VcompH2O=mxGetPr(prhs[8]);

    SvO2=input1[0];
    CvO2=input1[1];
    CvCO2=input1[2];
    CvN2=input1[3];
    CvGas5=input1[4];
    PvO2=input1[5];
    PvCO2=input1[6];
    PvN2=input1[7];
    PvGas5=input1[8];
    pHv=input1[9];
    HCO3v=input1[10];

    for (i=0;i<6;i++) {
        plhs[i] = mxCreateDoubleMatrix(1, Ncomp, mxREAL);
    }

    outO2c=mxGetPr(plhs[0]);
    outCO2c=mxGetPr(plhs[1]);
    outN2c=mxGetPr(plhs[2]);
    outGas5c=mxGetPr(plhs[3]);
    outPalvO2= mxGetPr(plhs[4]);
    outPccapO2=mxGetPr(plhs[5]);
```

After solution

	A.mat	patient.mat
Original Simulation	259.1 s	51 s
C in jupyterlab on Ubuntu	48.2 s	9.98 s
C in jupyterlab on DEEP	108.8 s	23.1 s

```
Rank 1 of 48 finished simulation in 22.27752375602722 seconds. Total run time was 46.93496060371399 seconds.
Rank 2 of 48 finished simulation in 43.93392872810364 seconds. Total run time was 72.65907120704651 seconds.
Rank 3 of 48 finished simulation in 44.01785612106323 seconds. Total run time was 73.29914355278015 seconds.
Rank 4 of 48 finished simulation in 43.18162775039673 seconds. Total run time was 71.32751655578613 seconds.
Rank 5 of 48 finished simulation in 44.13146686553955 seconds. Total run time was 72.40259027481079 seconds.
Rank 6 of 48 finished simulation in 43.0733118057251 seconds. Total run time was 70.90672993659973 seconds.
Rank 7 of 48 finished simulation in 44.137219190597534 seconds. Total run time was 73.81737112998962 seconds.
Rank 8 of 48 finished simulation in 43.43659210205078 seconds. Total run time was 71.90561842918396 seconds.
Rank 9 of 48 finished simulation in 44.07509183883667 seconds. Total run time was 73.38013052940369 seconds.
Rank 10 of 48 finished simulation in 41.9180543422699 seconds. Total run time was 69.32070708274841 seconds.
Rank 11 of 48 finished simulation in 44.34493088722229 seconds. Total run time was 73.59664535522461 seconds.
Rank 12 of 48 finished simulation in 40.76093912124634 seconds. Total run time was 67.81874299049377 seconds.
Rank 13 of 48 finished simulation in 44.04361939430237 seconds. Total run time was 72.92969369888306 seconds.
Rank 14 of 48 finished simulation in 28.152547359466553 seconds. Total run time was 55.31520986557007 seconds.
Rank 15 of 48 finished simulation in 44.230467557907104 seconds. Total run time was 73.9735004901886 seconds.
Rank 16 of 48 finished simulation in 43.04027509689331 seconds. Total run time was 71.08016061782837 seconds.
Rank 17 of 48 finished simulation in 26.79906988143921 seconds. Total run time was 53.50450015068054 seconds.
Rank 18 of 48 finished simulation in 25.79296875 seconds. Total run time was 52.27118730545044 seconds.
Rank 19 of 48 finished simulation in 44.080771684646606 seconds. Total run time was 73.71483135223389 seconds.
Rank 20 of 48 finished simulation in 41.73061966896057 seconds. Total run time was 68.9439389705658 seconds.
Rank 21 of 48 finished simulation in 44.19754076004028 seconds. Total run time was 73.24355792999268 seconds.
Rank 22 of 48 finished simulation in 26.41041898727417 seconds. Total run time was 53.03510904312134 seconds.
Rank 23 of 48 finished simulation in 44.16228485107422 seconds. Total run time was 73.05668640136719 seconds.
Rank 24 of 48 finished simulation in 43.1807427406311 seconds. Total run time was 70.12619829177856 seconds.
Rank 25 of 48 finished simulation in 29.01823616027832 seconds. Total run time was 68.62715768814087 seconds.
Rank 26 of 48 finished simulation in 59.97728204727173 seconds. Total run time was 98.74762678146362 seconds.
Rank 27 of 48 finished simulation in 60.527398109436035 seconds. Total run time was 100.05423736572266 seconds.
Rank 28 of 48 finished simulation in 60.1021511554718 seconds. Total run time was 99.16633081436157 seconds.
Rank 29 of 48 finished simulation in 60.539443254470825 seconds. Total run time was 100.36254119873047 seconds.
Rank 30 of 48 finished simulation in 59.01609516143799 seconds. Total run time was 97.88020157814026 seconds.
Rank 31 of 48 finished simulation in 60.67410683631897 seconds. Total run time was 99.81805229187012 seconds.
Rank 32 of 48 finished simulation in 60.6573441028595 seconds. Total run time was 100.60840487480164 seconds.
Rank 33 of 48 finished simulation in 60.693350076675415 seconds. Total run time was 100.79338216781616 seconds.
Rank 34 of 48 finished simulation in 58.74378705024719 seconds. Total run time was 97.4392876625061 seconds.
Rank 35 of 48 finished simulation in 60.43499994277954 seconds. Total run time was 99.917888879776 seconds.
Rank 36 of 48 finished simulation in 60.43606972694397 seconds. Total run time was 100.20979976654053 seconds.
Rank 37 of 48 finished simulation in 60.20894169807434 seconds. Total run time was 99.54638195037842 seconds.
Rank 38 of 48 finished simulation in 57.83604335784912 seconds. Total run time was 96.76804447174072 seconds.
Rank 39 of 48 finished simulation in 60.768128395080566 seconds. Total run time was 100.96197700500488 seconds.
Rank 40 of 48 finished simulation in 60.819724559783936 seconds. Total run time was 100.84107732772827 seconds.
Rank 41 of 48 finished simulation in 43.65770959854126 seconds. Total run time was 83.34533095359802 seconds.
Rank 42 of 48 finished simulation in 57.3722665309906 seconds. Total run time was 96.19882464408875 seconds.
Rank 43 of 48 finished simulation in 60.36100220680237 seconds. Total run time was 99.64496517181396 seconds.
Rank 44 of 48 finished simulation in 58.68684673309326 seconds. Total run time was 97.71003341674805 seconds.
Rank 45 of 48 finished simulation in 59.40385913848877 seconds. Total run time was 98.80751347541809 seconds.
Rank 46 of 48 finished simulation in 55.70101356506348 seconds. Total run time was 94.33447027206421 seconds.
Rank 47 of 48 finished simulation in 59.21916604042053 seconds. Total run time was 98.42237854003906 seconds.
Rank 48 of 48 finished simulation in 60.588436126708984 seconds. Total run time was 100.46083521842957 seconds.
```

Thank you for your attention