

Hellow,

I found two flaws.

1. Four Lagrangian interpolation functions in namespace Polylib may have significant errors when evaluation near interpolation points. This problem affects interpolation operations' accuracy.

These four functions are the follows:

double hgj (const int i, const double z, const double *zgj, const int np, const double alpha, const double beta),

double hgrjm (const int i, const double z, const double *zgrj, const int np, const double alpha, const double beta),

double hgrjp (const int i, const double z, const double *zgrj, const int np, const double alpha, const double beta),

double hglj (const int i, const double z, const double *zglj, const int np, const double alpha, const double beta).

The reason of this problems is this. These four functions using formulas like this one

$$h_j(z) = \begin{cases} \frac{(1-z^2)P_{np-2}^{\alpha+1,\beta+1}(z)}{((1-z_j^2)[P_{np-2}^{\alpha+1,\beta+1}(z_j)]' - 2z_j P_{np-2}^{\alpha+1,\beta+1}(z_j))(z-z_j)} & \text{if } z \neq z_j \\ 1 & \text{if } z = z_j \end{cases},$$

used in hglj. To judge whether z equals z_j , a parameter $\text{EPS} = 100 * \text{DBL_EPSILON}$ is adopted as a threshold, and $\text{EPS} = 2.E-14$. Problem happens when z is very close to z_j but their distance is still greater than EPS, since at this situation the formula in h_j contains subtraction of two very close (double) float numbers, which causes heavy loss of accuracy.

One example is in Gauss Lobatto interpolation function hglj with $n=12$, I evaluate its value at point -0.81927932164452633 , which differs from the third zero -0.81927932164400674 by $5E-13 > \text{EPS}$. Function hglj gives the value 1.00015479671952878 , of which the error is $1E-4$.

I use a new parameter $\text{EPSERR} = 3E-3$ as threshold specially for these four functions to judge whether z is close to z_j enough, and if $\text{abs}(z-z_j) < \text{EPSERR}$, I adopt a traditional Lagrange interpolation function $h_j(z) = \prod_{\substack{0 \leq m < n \\ m \neq j}} \frac{z-z_m}{z_j-z_m}$ to evaluate its value. This gives a very good overall accuracy.

2. In function Nektar::FieldUtils::InputXml::Process ,the “if” statement at line 356 version 4.4.0. I think it should be this `if(m_requireEquiSpaced)` but not `if(m_requireEquiSpaced || vm.count("output-points"))`. Since in the current codes, when `--output-points` and `--noequispaced` options are used simultaneously, the `--equispaced` option will not work.

And still, I have a question. In function Nektar::Extrapolate::AccelerationBDF when solving incompressible Navier-Stokes equation using higher order Neumann pressure boundary condition, why should the backward differentiation formula start after `m_pressureCalls > 2`? since when `m_pressureCalls=2`, we can already obtain a first order accuracy value of $\frac{\partial u}{\partial t}$. I changed that number to 1, like the following codes

```
if (m_pressureCalls > 1)
{
    int acc_order = min(m_pressureCalls-1,m_intSteps); ...
```

and it seems nothing goes wrong in my simulation.

Best wishes

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