

COQ-862 – Métodos numéricos para sistemas distribuídos

Teoria do funcional da densidade dinâmica aplicada
a adsorção em microporo por volumes finitos

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SUMÁRIO DA APRESENTAÇÃO

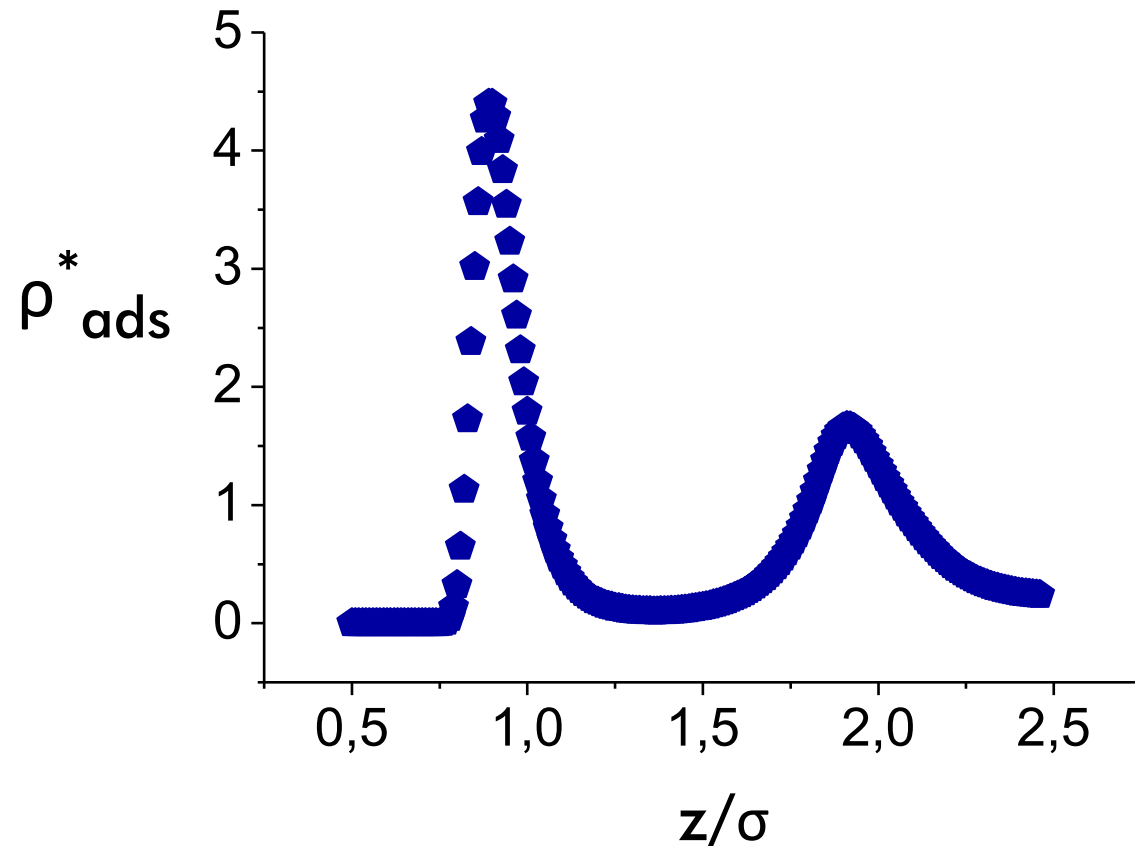
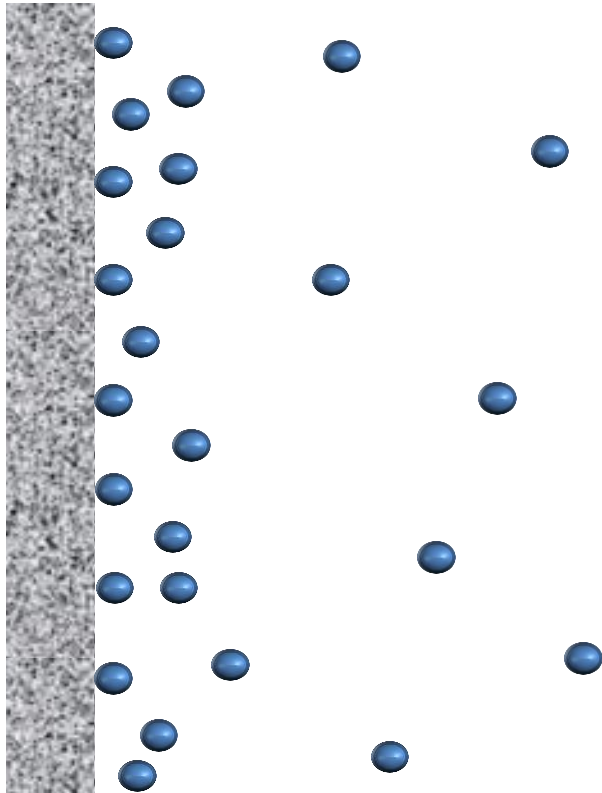
- **Introdução**
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- **Resultados**
- **Conclusão**
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INTRODUÇÃO



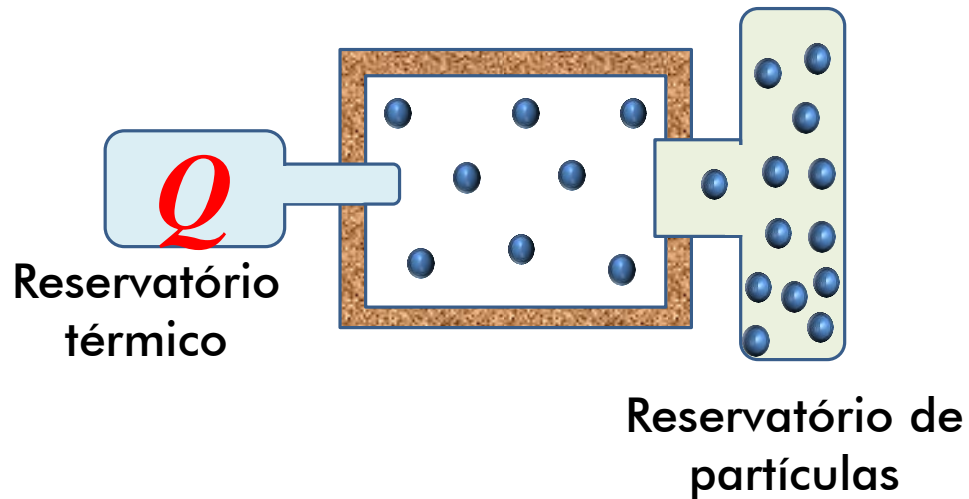
ADSORÇÃO

AUMENTO DA DENSIDADE DOS COMPONENTES DE UM FLUIDO NA VIZINHANÇA DE UMA INTERFACE



PROPRIEDADES TERMODINÂMICAS DO SISTEMA – A PARTIR DA DFT

ensemble grande canônico
 $\Omega(\mu, V, T)$



Cálculo da densidade
no equilíbrio

$$\left[\frac{\delta \Omega[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})} = 0 \right]$$

$$\frac{\delta \Omega[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})} = \frac{\delta F[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})} - (\mu)$$

$$\frac{\delta F[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})} = \mu$$

DDFT – TEORIA DO FUNCIONAL DA DENSIDADE DINÂMICA




A dinâmica é tratada como uma migração pontos equilíbrios locais

$$\frac{\delta F[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})} = \mu$$

DDFT – TEORIA DO FUNCIONAL DA DENSIDADE DINÂMICA

$$\frac{\partial \rho(r, t)}{\partial t} = \nabla \cdot j(r, t)$$

$$\frac{\partial \rho(r, t)}{\partial t} = \nabla \cdot \left(\Gamma \rho(r, t) \nabla \frac{\delta F[\rho]}{\delta \rho(r, t)} \right)$$



Ao considerar
perto do
equilíbrio

METODOLOGIA |

ENERGIA LIVRE FOI APROXIMADA PELA SOMA DOS TERMOS DE IDEALIDADE E POTENCIAL EXTERNO

$$F = F_{ideal} + F_{externo}$$

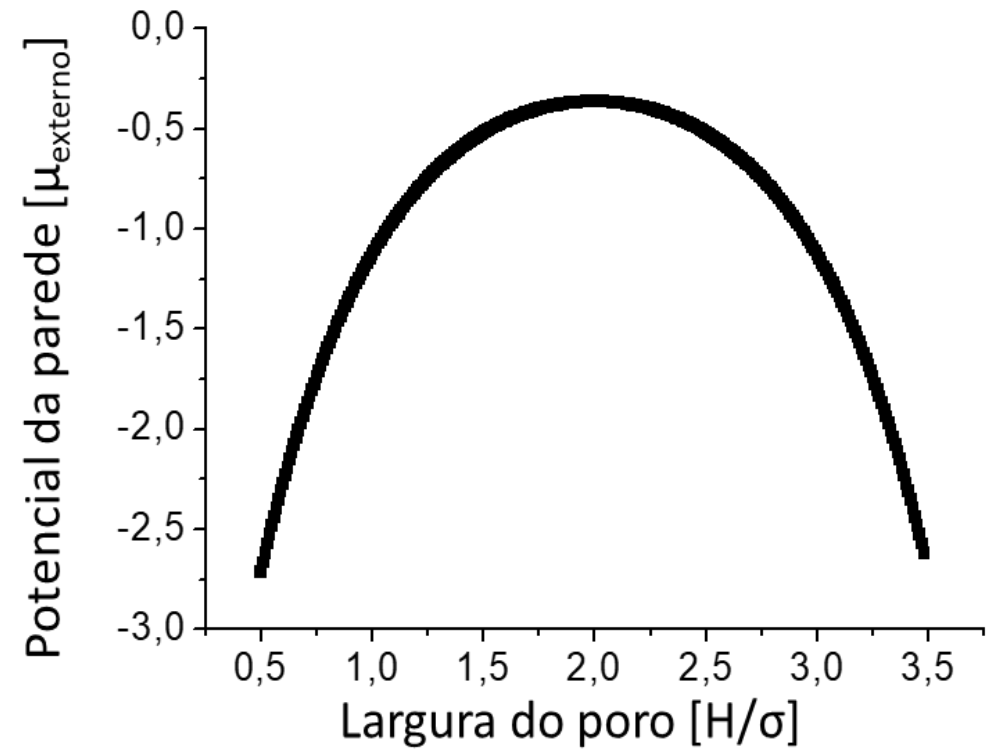
$$\frac{\delta F_{ideal}[\rho]}{\delta \rho} = k_B T \ln(\rho(r, t))$$

$$\frac{\delta F_{externo}[\rho]}{\delta \rho} = \frac{\delta \int dr \rho(r, t) \cdot V_{ext}(r)}{\delta \rho} = V_{ext}(r)$$

POTENCIAL EXTERNO INDUZIDO PELAS PAREDES

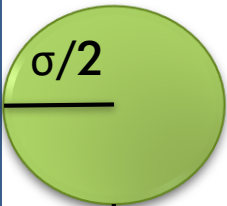
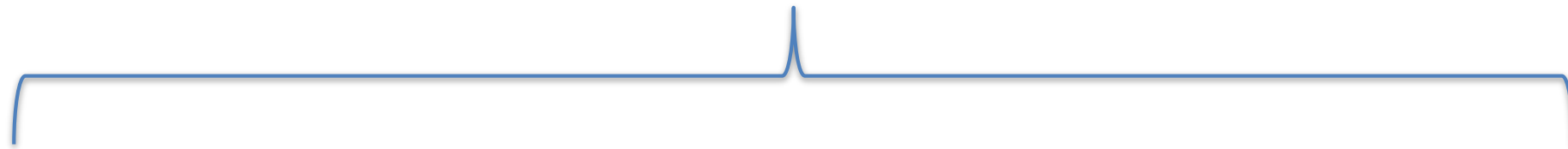
$$V_{ext}(z) = \phi(z) + \phi(H - z)$$

$$\phi(z) = -2 * \exp\left(-1.8 * \left(z - \frac{\sigma}{2}\right)\right) / T$$



Modelo de poro do tipo Fenda

Volumes Finitos

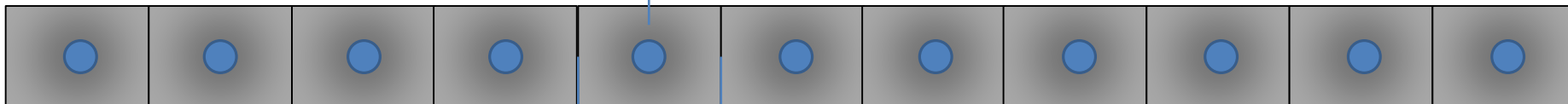


$\sigma/2$

Distância
de $\sigma/2$



Pontos nodais

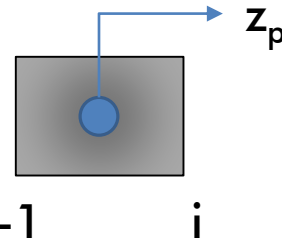


Pontos nas faces

$$\int_{i-1}^i \frac{\partial \rho(z, t)}{\partial t} dz = \int_{i-1}^i \frac{\partial}{\partial z} \cdot \left(\rho(z, t) \frac{\partial \mu}{\partial z} \right) dz$$

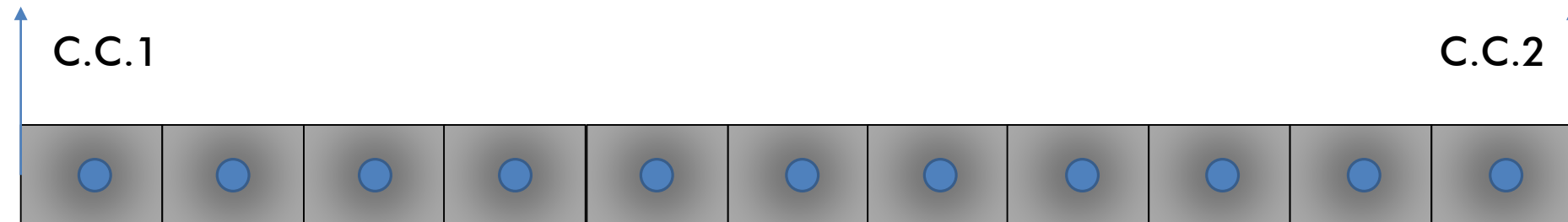
$$\frac{d\rho_p(t)}{dt} = \frac{1}{\Delta z} \left(\rho \frac{\partial \mu}{\partial z} \right) \Big|_{i-1}^i$$

Integrado no volume finito



Fluxo zerado
Na primeira face

Fluxo zerado
Na última face



Condição inicial

$$\rho_0 = 1.50060829911943E-06$$

Constante

z

Acessado em:

<http://web.media.mit.edu/~crtaylor/calculator.html>

Finite Difference Coefficients Calculator

What is this?

Locations of Sampled Points

-1.5,-0.5,0.5,1.5]

Derivative Order

1

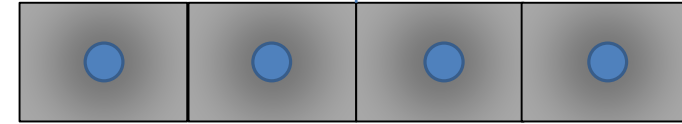
Finite Difference Equation

$$\frac{\partial^{(1)}f}{\partial x^{(1)}} \approx \frac{1f(x - 1.5h) - 27f(x - 0.5h) + 27f(x + 0.5h) - 1f(x + 1.5h)}{24h^1}$$

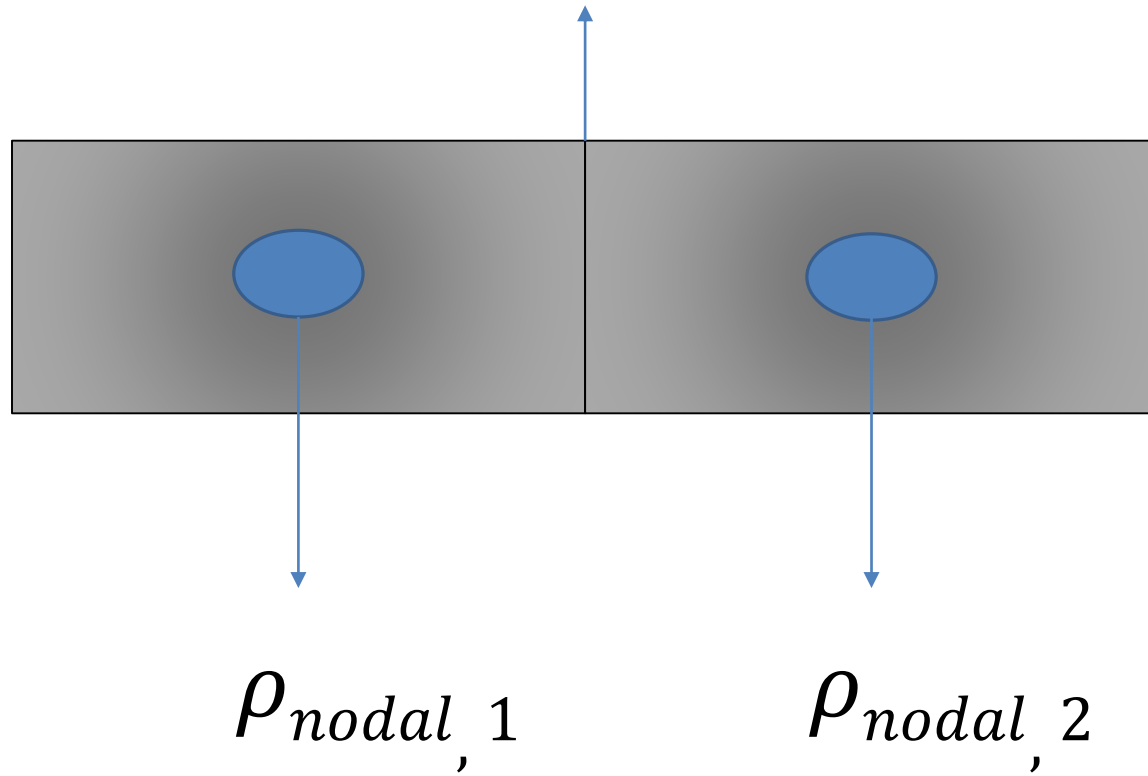
Python Code

```
f_x = (1*f[i-1.5]-27*f[i-0.5]+27*f[i+0.5]-1*f[i+1.5])/(24*1.0*h**1)
```

How does it work?



$$\rho_{face} = \frac{\rho_{nodal,1} + \rho_{nodal,2}}{2}$$



INTEGRADORES TEMPORAIS EMPREGADOS

- Euler explícito
- Runge-Kutta 4ª ordem (explícito)
- DASSL

Análise temporal $dt = 1,0e-8$

RESULTADOS

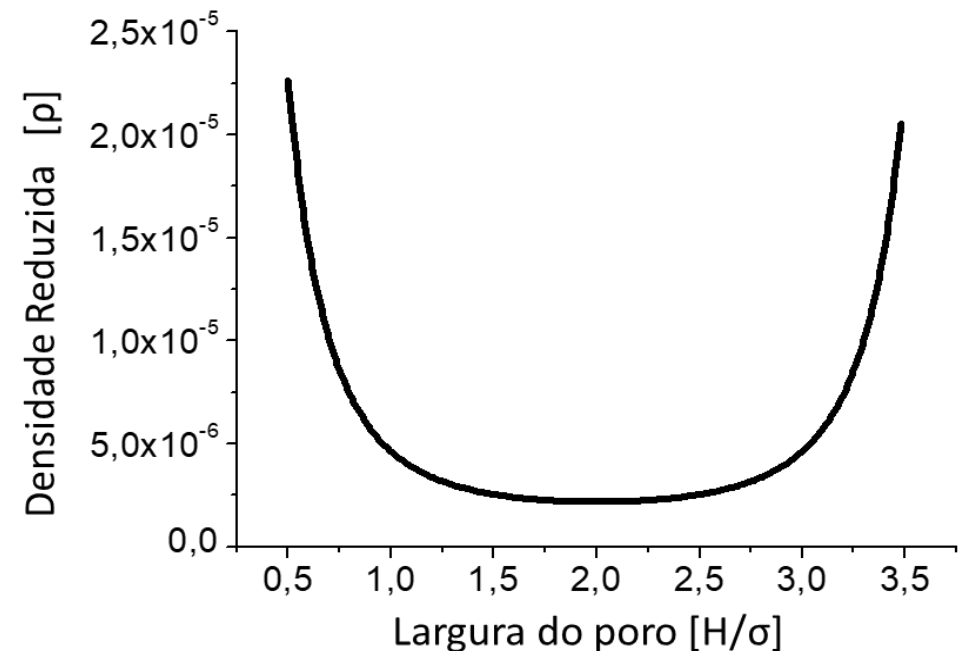


OTIMIZAÇÃO DA MALHA – ERRO RELATIVO < 1%

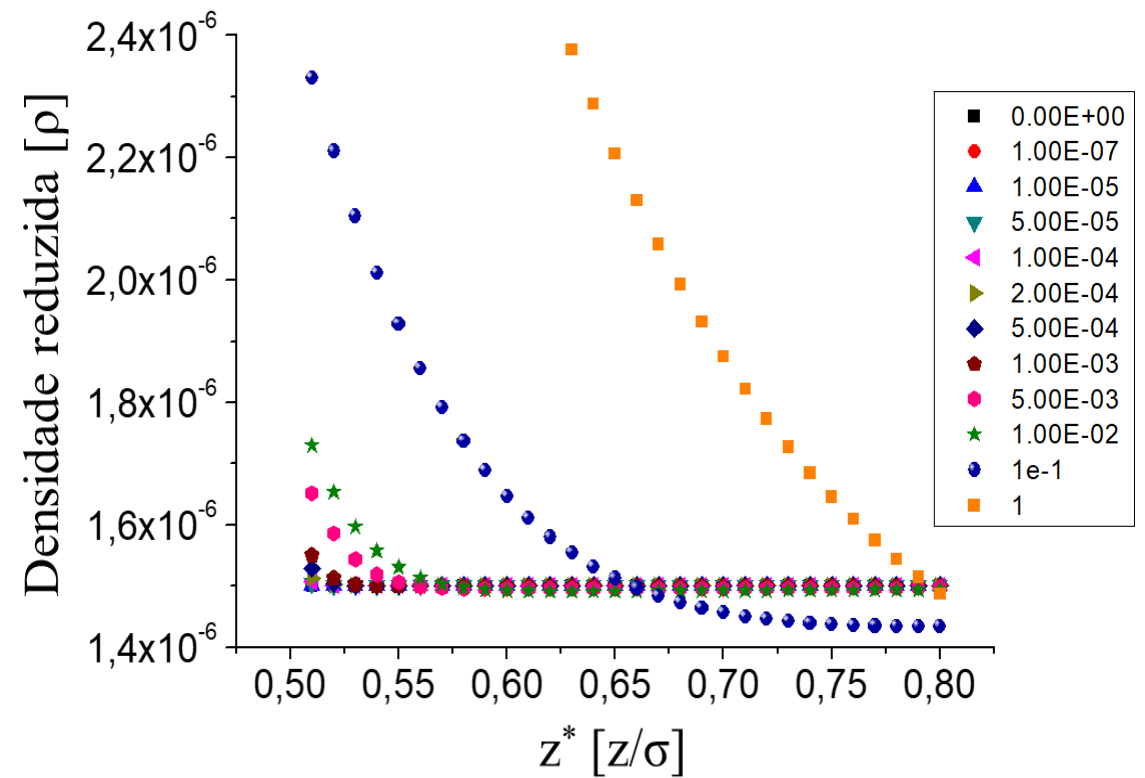
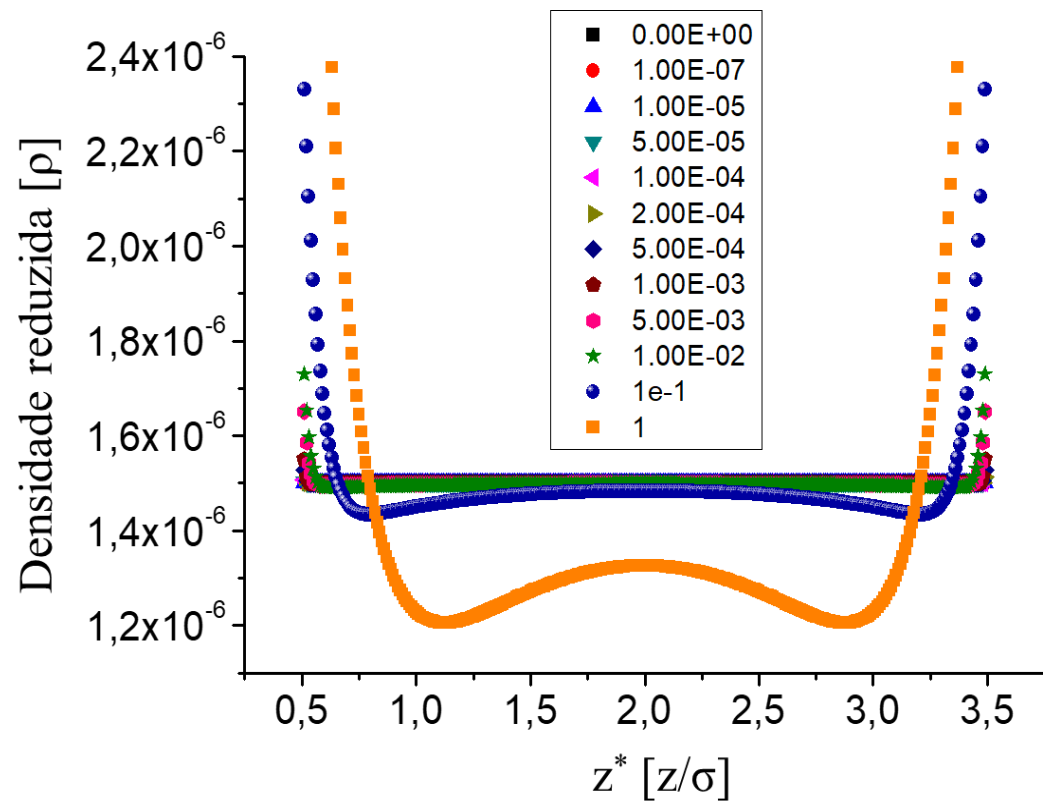
Teste de diferentes malhas

dz	np	Ads	Erro relativo
0,008	500	1,51590E-05	0,5921%
0,010	400	1,52493E-05	2,6139%
0,020	200	1,48608E-05	6,9788%
0,080	50	1,38914E-05	8,7649%
0,100	40	1,27719E-05	

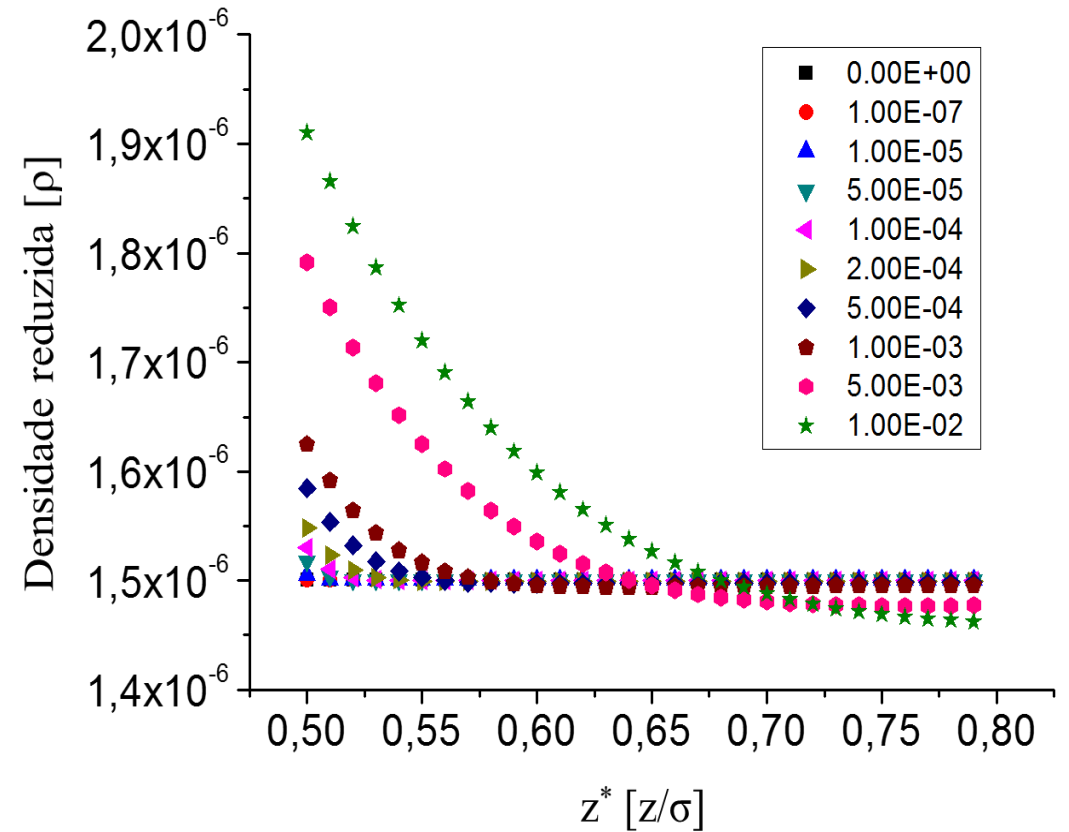
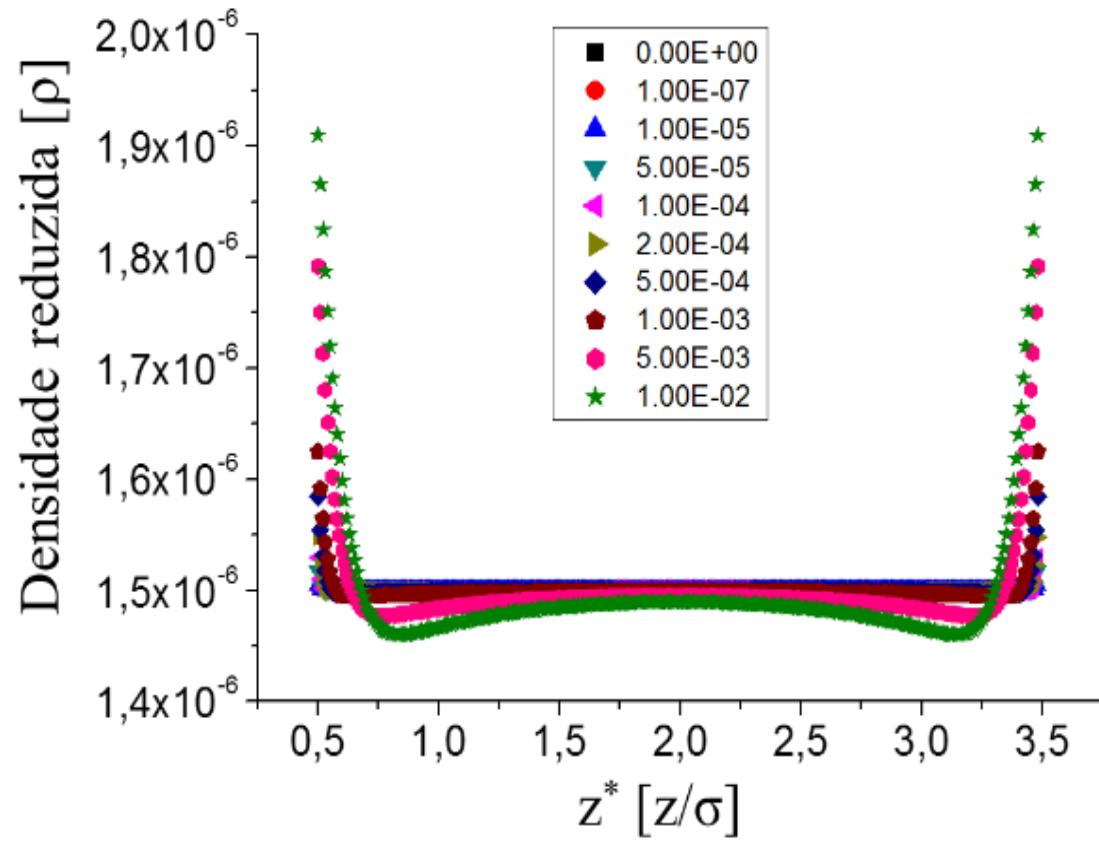
$$Ads = \int \rho dz$$



EULER EXPLÍCITO



RUNGE-KUTTA 4ª ORDEM (EXPLÍCITO)



DASSL PARA TEMPOS $> 4E-3$

```
!INICIANDO OS PARÂMETROS DA DASSL
T=0.D0                !TEMPO ATUAL (TEMPO INICIAL NESSE CASO)
DT=1.D-8
TEND=5.D-3
do i=1,nup
  Y(i)=
enddo

TOUT=T+DT
INFO=0
info(2) =
RTOL=1.D-6
ATOL=1.D-8
NEQ=299
LIW=319
LRW=92132
!PASSAGEM
DASSL-- AT T (<=R1) SOME ELEMENT OF WT
          In above message, R1 = 0.4026531830000E-02
DASSL-- HAS BECOME .LE. 0.0
          -3
Fortran Pause - Enter command<CR> or <CR> to continue.

RPAR(1)=Te
RPAR(2)=0.
RPAR(3)=La
RPAR(4)=dz
IPAR(1)=nup
```

- ✓ Previsão da dinâmica de adsorção - molécula ideal / poro do tipo fenda
- ✓ Otimização da malha – $0,01\sigma$
- ✓ Implementação com sucesso dos métodos de Euler e Runge-Kutta para o cálculo de DDFT
- ✓ Necessidade de revisão do código com o algoritmo DASSL

CONCLUSÕES



OBRIGADO

REFERÊNCIAS

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