Domain Decomposition Methods for the Poisson-Boltzmann Equations

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Joint work with B. Stamm (Universität Stuttgart, Stuttgart)

Outline

- Ionic Solvation Models [1]
  - Explicit Solvation Models
    - Adopts molecular representation of both solute and solvent
    - Accurate results
    - Computationally expensive

[1] Zhang et. al.: JCTC, 13, 1034-1043, 2017

[2] Cances, Mennucci, Tomasi: JCP 107 (8), 3032-3041, 1997

[3] Honig, Nicholls: Sci. 268, 1144-1149, 1995

- Ionic Solvation Models [1]
  - Explicit Solvation Models
    - Adopts molecular representation of both solute and solvent
    - Accurate results
    - Computationally expensive
  - Implicit Solvation Models [2,3]
    - Microscopic treatment of solute
    - Macroscopic treatment of solvent using physical properties
    - Less computational cost

[1] Zhang et. al.: JCTC, 13, 1034-1043, 2017

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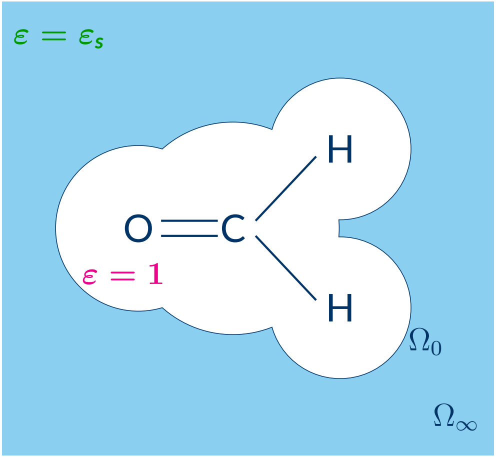

Figure 1: Formaldehyde Molecule

- Poisson-Boltzman (PB) Equation [1,2]

$$-\nabla \cdot \left[\varepsilon_{\text{abs}}\varepsilon(\mathbf{x})\nabla\tilde{\psi}(\mathbf{x})\right] = \rho^{\text{sol}}(\mathbf{x}) + \rho^{\text{ions}}(\mathbf{x}) \quad \text{in } \mathbb{R}^3$$

  - $\tilde{\psi}(\mathbf{x})$: Electrostatic potential

[1] Gouy: JPTA 9, 457-468, 1910

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  - $\tilde{\psi}(\mathbf{x})$: Electrostatic potential
  - $\varepsilon(\mathbf{x})$: Space-dependent dielectric permittivity
  - $\rho^{\text{sol}}(\mathbf{x})$: Solute charge distribution

$$\rho^{\text{sol}}(x) = \sum_{i=1}^{M} q_i \delta(\mathbf{x} - \mathbf{x}_i)$$

  - M : Number of solute atoms
  - q_i : Total charge on the i^{th} atom

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- $\rho^{\text{ions}}(\mathbf{x})$: Ionic charge distribution

$$\rho^{\text{ions}}(\mathbf{x}) = \sum_{i=1}^{N_{\text{ions}}} z_i e \lambda(\mathbf{x}) c_i^{\infty} \exp\left(\frac{-z_i e \tilde{\psi}(\mathbf{x})}{K_B T}\right)$$

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- For $1:1$ ionic solution[1]

$$\rho^{\text{ions}}(\mathbf{x}) = -2ce\lambda(\mathbf{x}) \sinh\left(\frac{e\tilde{\psi}(\mathbf{x})}{K_B T}\right)$$

  - $\lambda(\mathbf{x})$: Ion-exclusion function

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[1] Debye, Hückel: PZ 24(9), 185-206, 1923

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- Dimensionless Poisson-Boltzman (PB) Equation

$$-\nabla \cdot \left[\varepsilon(\mathbf{x}) \nabla \psi(\mathbf{x})\right] + \kappa^2 \varepsilon_{\mathsf{s}} \lambda(\mathbf{x}) \sinh\left(\psi(\mathbf{x})\right) = \frac{1}{\beta \varepsilon_{\mathsf{abs}}} \rho^{\mathsf{sol}}(\mathbf{x}) \quad \text{in } \mathbb{R}^3$$

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- For $1:1$ solution Poisson-Boltzman (PB) Equation

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  - $\psi(\mathbf{x}) : \tilde{\psi}(\mathbf{x})\beta$
  - κ : Debye Hückel Screening Constant [1]
  - β : $e/K_{\mathrm{B}}T$

[1] Debye, Hückel: PZ 24(9), 185-206, 1923

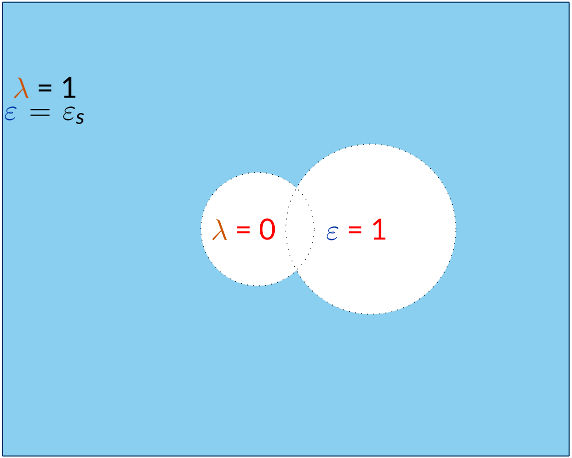
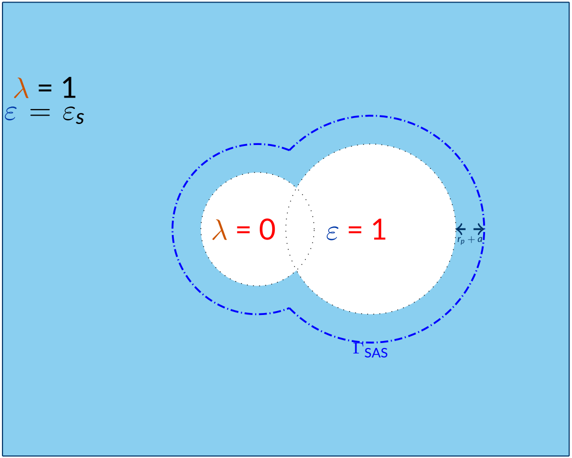


Figure 2: Solute probes and solute-solvent boundary for a molecule



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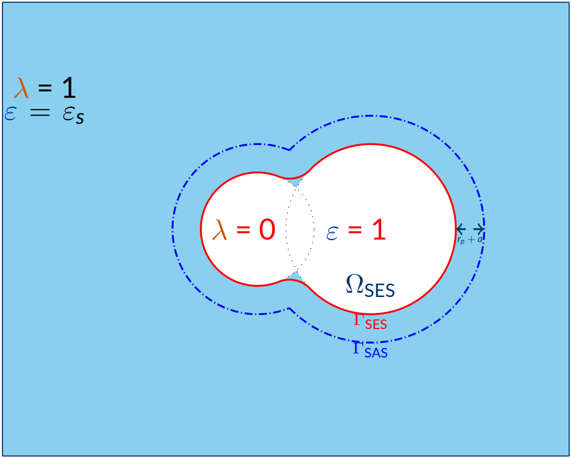

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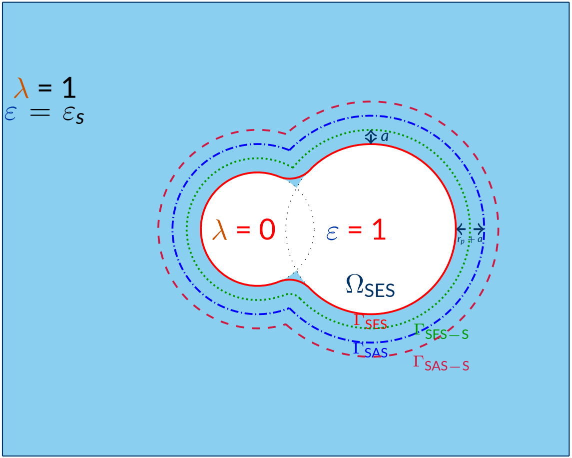

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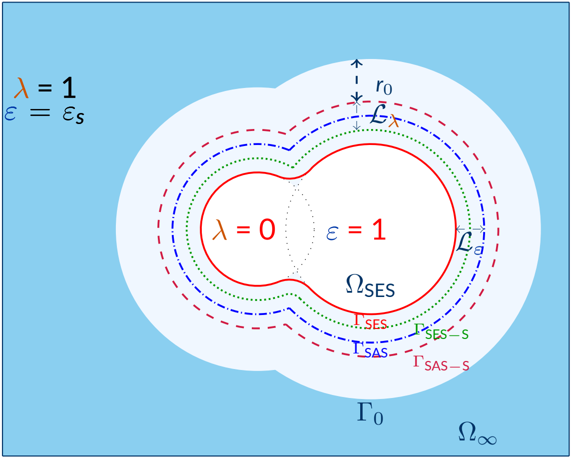

Figure 2: Solute probes and solute-solvent boundary for a molecule

- Dielectric Permittivity Function[1]

$$\varepsilon(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in \Omega_{\mathsf{SES}}, \\ 1 + (\varepsilon_s - 1)\xi\left(\dfrac{f_{\mathsf{SAS}}(\mathbf{x}) + r_p + a}{r_p + a}\right) & \mathbf{x} \in \mathcal{L}_{\varepsilon}, \\ \varepsilon_s & \text{else}, \end{cases}$$

[1] Quan, Stamm: JCP, 322, 760-782, 2016

[2] Stern: ZFE, 30(21-22), 508, 1924

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- Ion-Exclusion Function[2]

$$\lambda(\mathbf{x}) = \begin{cases} 0 & \mathbf{x} \in \Omega_{\mathrm{SES-S}}, \\ \xi\left(\dfrac{f_{\mathrm{SAS}}(\mathbf{x}) + r_p}{r_p + a}\right) & \mathbf{x} \in \mathcal{L}_{\lambda}, \\ 1 & \text{else}, \end{cases}$$

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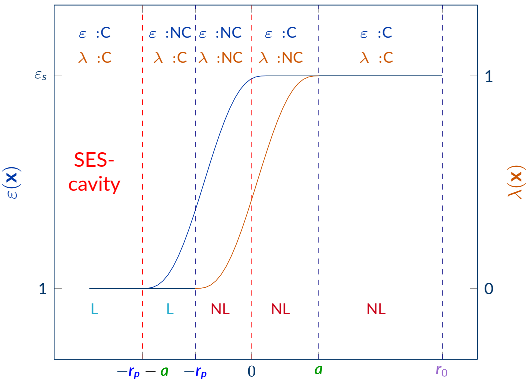
Linearity in Different Regions



- C: Constant, NC: Non-Constant
- L: Linear, NL: Non-Linear

- The PB equation can be written in two equations

$$
\begin{aligned}
-\nabla\cdot[\varepsilon(\mathbf{x})\nabla\psi(\mathbf{x})]+\kappa^2\varepsilon_{\mathsf{s}}\lambda(\mathbf{x})\sinh(\psi(\mathbf{x})) &= \frac{1}{\beta\varepsilon_{\mathsf{abs}}}\rho^{\mathsf{sol}}(\mathbf{x}) && \text{in } \Omega_0,\\
-\Delta\psi(\mathbf{x})+\kappa^2\psi(\mathbf{x}) &= 0 && \text{in } \Omega_\infty,
\end{aligned}
$$

with

$$
\begin{aligned}
[\![\psi]\!] &= 0,\\
[\![\partial_{\mathbf{n}}\psi]\!] &= 0 \quad \text{on} \quad \Gamma_0 := \partial\Omega_0,
\end{aligned}
$$

- Using Potential Theory the final equations are

$$
\begin{aligned}
-\nabla \cdot \left[\varepsilon(\mathbf{x})\nabla\psi_{\mathsf{r}}(\mathbf{x})\right] + \kappa^2\varepsilon_{\mathsf{s}}\lambda(\mathbf{x})\mathcal{F}\left(\psi_{\mathsf{r}}+\psi_0\right)\left(\psi_{\mathsf{r}}+\psi_0\right)(\mathbf{x}) \\
= \nabla \cdot \left[\left(\varepsilon(\mathbf{x})-1\right)\nabla\psi_0(\mathbf{x})\right] \qquad \text{in } \Omega_0 \qquad \text{[GSP]}
\end{aligned}
$$

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\end{aligned}
$$

$$
-\Delta\psi_{\mathsf{e}}(\mathbf{x}) + \kappa^2\psi_{\mathsf{e}}(\mathbf{x}) = 0 \quad \text{in } \Omega_0 \quad \text{[HSP]}
$$

- Using Potential Theory the final equations are

$$-\nabla \cdot [\varepsilon(\mathbf{x})\nabla\psi_{\mathsf{r}}(\mathbf{x})] + \kappa^2\varepsilon_{\mathsf{s}}\lambda(\mathbf{x})\mathcal{F}\left(\psi_{\mathsf{r}} + \psi_0\right)\left(\psi_{\mathsf{r}} + \psi_0\right)(\mathbf{x}) = \nabla \cdot [(\varepsilon(\mathbf{x}) - 1)\nabla\psi_0(\mathbf{x})] \quad \text{in } \Omega_0 \qquad \text{[GSP]}$$

$$-\Delta\psi_{\mathsf{e}}(\mathbf{x}) + \kappa^2\psi_{\mathsf{e}}(\mathbf{x}) = 0 \quad \text{in } \Omega_0 \qquad \text{[HSP]}$$

with

$$\begin{aligned} \psi_0 + \psi_{\mathsf{r}} &= \psi_{\mathsf{e}} && \text{on } \Gamma_0, \\ \psi_{\mathsf{e}} &= S_\kappa\sigma_{\mathsf{e}} && \text{on } \Gamma_0 \end{aligned}$$

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$$
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\psi_{\mathrm{e}} &= S_\kappa \sigma_{\mathrm{e}} \quad \text{on } \Gamma_0
\end{aligned}
$$

where

- ψ_{r} : Reaction potential in Ω
- ψ_0 : Potential generated by ρ_{M} satisfying,

$$
-\Delta\psi_0 = \frac{1}{\beta\varepsilon_{\mathrm{abs}}}\rho_{\mathrm{M}}
$$

- ψ_{e} : Extended potential from Ω^{C} to Ω^0

[1] Sauter, Schwab, Springer, Berlin-2011, 101-181

- ψ_e : Extended potential from Ω^C to Ω^0
- $\mathcal{F}(\Phi) = \dfrac{\sinh(\Phi)}{\Phi}$

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- ψ_e : Extended potential from Ω^C to Ω^0
- $\mathcal{F}(\Phi) = \dfrac{\sinh(\Phi)}{\Phi}$
- σ_e : Charge density generating ψ_e satisfying

$$S_\kappa \sigma_e(\mathbf{x}) = \int_{\Gamma_0} \frac{\exp\left(-\kappa|\mathbf{x}-\mathbf{y}|\right)\sigma_e(\mathbf{y})}{4\pi|\mathbf{x}-\mathbf{y}|} = \psi_e \quad \forall\, \mathbf{x} \in \Gamma_0$$

- S_κ : Invertible single-layer potential operator [1]

$$S_\kappa : H^{-1/2}(\Gamma_0) \to H^{1/2}(\Gamma_0)$$

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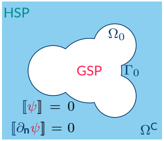
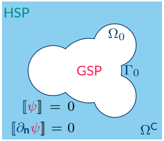
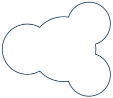
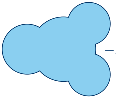

HSP
Ω_0
GSP
Γ_0
$[\![\psi]\!] = 0$
$[\![\partial_{\mathbf{n}}\psi]\!] = 0$
Ω^{C}

ddPB-Method



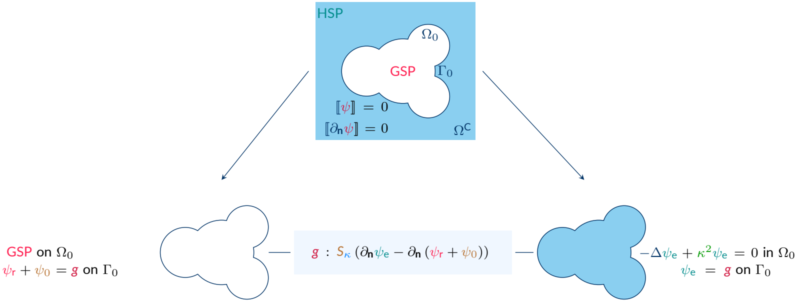
GSP on Ω_0
$\psi_r + \psi_0 = g$ on Γ_0





$$-\Delta \psi_e + \kappa^2 \psi_e = 0 \text{ in } \Omega_0$$
$$\psi_e = g \text{ on } \Gamma_0$$

ddPB-Method



HSP
Ω_0
GSP
Γ_0
$[\![\psi]\!] = 0$
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Ω^C
GSP on Ω_0
$\psi_r + \psi_0 = g$ on Γ_0
$g : S_\kappa(\partial_{\mathbf{n}}\psi_e - \partial_{\mathbf{n}}(\psi_r + \psi_0))$
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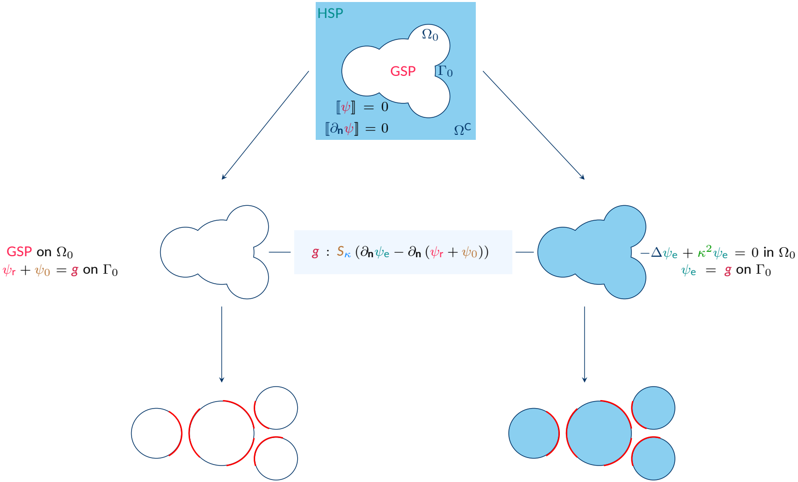
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- We can decompose Ω_0

$$\Omega_0 = \bigcup_{j=1}^{M} \Omega_j, \qquad \Omega_j = B_{R_j}(\mathbf{x}_j)$$

  - $R_j = r_j + a + r_0 + r_p$

[1] Cances, Maday, Stamm: JCP 139(5), 054111, 2013
[2] Lipparini, Stamm, Cances, Maday, Mennucci: JCTC 9(8), 3637-3648, 2013
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[4] Stamm, Cances, Lipparini, Maday: JCP 144, 054101, 2016
[5] Gatto, Lipparini, Stamm: JCP 147, 224108, 2017
[6] Quan, Stamm, Maday: SISC 41(2), B320-B350, 2019
[7] J., Nottoli, Mikhalev, Quan, Stamm: JCP 158, 104105, 2023
[8] Nottoli, Herbst, J., Lipparini, Mikhalev, Stamm: ddX: https://github.com/ddsolvation/ddX

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- History of dd-methods
  - ddCOSMO: COnductor-like Screening MOdel[1,2,3]

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- GSP equation in unit ball

$$
\begin{aligned}
-\nabla\cdot\left[\tilde{\varepsilon}(\mathbf{x})\nabla u(\mathbf{x})\right]+\tilde{\lambda}(\mathbf{x})\tilde{\mathcal{F}}\left(\overline{u}(\mathbf{x})\right)u(\mathbf{x}) &= f(\mathbf{x}) && \text{in } B_1(\mathbf{0})\\
u(\mathbf{x}) &= \phi_{\mathrm{r}}(\mathbf{x}) && \text{on } \partial B_1(\mathbf{0})
\end{aligned}
$$

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$$
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u(\mathbf{x}) &= \phi_{\mathrm{r}}(\mathbf{x}) \quad \text{on} \quad \partial B_1(\mathbf{0})
\end{aligned}
$$

- Transformation to Homogeneous Problem

$$
\begin{aligned}
-\nabla \cdot [\tilde{\varepsilon}(\mathbf{x})\nabla w(\mathbf{x})] + \tilde{\lambda}(\mathbf{x})\tilde{\mathcal{F}}\left(\left(\overline{w + \hat{u}_1}\right)(\mathbf{x})\right) w(\mathbf{x}) &= \tilde{f}(\mathbf{x}), \quad \text{in} \quad B_1(\mathbf{0}) \\
w(\mathbf{x}) &= 0 \quad \text{on} \quad \partial B_1(\mathbf{0}),
\end{aligned}
$$

- GSP equation in unit ball

$$\begin{aligned} -\nabla \cdot [\tilde{\varepsilon}(\mathbf{x})\nabla u(\mathbf{x})] + \tilde{\lambda}(\mathbf{x})\tilde{\mathcal{F}}(\overline{u}(\mathbf{x}))\, u(\mathbf{x}) &= f(\mathbf{x}) \quad \text{in} \quad B_1(\mathbf{0}) \\ u(\mathbf{x}) &= \phi_{\mathrm{r}}(\mathbf{x}) \quad \text{on} \quad \partial B_1(\mathbf{0}) \end{aligned}$$

- Transformation to Homogeneous Problem

$$\begin{aligned} -\nabla \cdot [\tilde{\varepsilon}(\mathbf{x})\nabla w(\mathbf{x})] + \tilde{\lambda}(\mathbf{x})\tilde{\mathcal{F}}\left(\left(\overline{w + \hat{u}_1}\right)(\mathbf{x})\right) w(\mathbf{x}) &= \tilde{f}(\mathbf{x}), \qquad \text{in} \ B_1(\mathbf{0}) \\ w(\mathbf{x}) &= 0 \qquad \text{on} \ \partial B_1(\mathbf{0}), \end{aligned}$$

  - $w(\mathbf{x}) = u(\mathbf{x}) - \hat{u}_1(\mathbf{x})$
  - $\tilde{f}(\mathbf{x}) = f(\mathbf{x}) + \nabla \cdot [\tilde{\varepsilon}(\mathbf{x})\nabla \hat{u}_1(\mathbf{x})] - \tilde{\lambda}(\mathbf{x})\tilde{\mathcal{F}}\left(\left(\overline{w + \hat{u}_1}\right)(\mathbf{x})\right) \hat{u}_1(\mathbf{x})$

- GSP equation in unit ball

$$
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  - $\psi_{\mathsf{r}}(\mathbf{x})$ is harmonic in $B_{r_j}(\mathbf{x}_j)$
  - $w(\mathbf{x})$ is harmonic in $B_{\delta}(\mathbf{0})$ where

$$\delta = \frac{r_j}{r_j + r_0 + r_p + a} \in (0,1)$$

- Find $w \in H^1_{0,\delta}(\mathcal{D})$ such that

$$\int_{\mathcal{D}} \tilde{\varepsilon}(\mathbf{x}) \nabla w(\mathbf{x}) \nabla \tilde{w}(\mathbf{x}) + \int_{\mathcal{D}} \tilde{\lambda}(\mathbf{x}) \tilde{\mathcal{F}}\left(\overline{w}(\mathbf{x})\right) w(\mathbf{x}) \tilde{w}(\mathbf{x}) + \int_{\partial B_\delta(\mathbf{0})} (\mathcal{T} w)\, \tilde{w}(\mathbf{x}) = \int_{\mathcal{D}} \tilde{f}(\mathbf{x}) \tilde{w}(\mathbf{x}) \quad \forall\ \tilde{w} \in H^1_{0,\delta}(\mathcal{D}),$$

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$$+ \int_{\partial B_\delta(\mathbf{0})} \left(\mathcal{T} w\right) \tilde{w}(\mathbf{x}) = \int_{\mathcal{D}} \tilde{f}(\mathbf{x}) \tilde{w}(\mathbf{x}) \quad \forall \ \tilde{w} \in H^1_{0,\delta}(\mathcal{D}),$$

  - $\mathcal{D} = B_1(\mathbf{0}) \setminus B_\delta(\mathbf{0})$
  - $H^1_{0,\delta}(\mathcal{D}) = \left\{ w \in H^1(\mathcal{D}) : w|_{\partial B_1(\mathbf{0})} = 0 \right\}$

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- Using Galerkin discretisation

$$w_{\mathcal{B}}(r,\theta,\varphi) = \sum_{i=0}^{N}\sum_{\ell=0}^{\ell_{\max}}\sum_{m=-\ell}^{\ell} [\phi_r]_{i\ell}^m\, \varrho_i(r) Y_\ell^m(\theta,\varphi) \quad \forall\ \delta \le r \le 1; \quad 0 \le \theta \le \pi; \quad 0 \le \varphi \le 2\pi,$$

  - ϱ_i : Legendre polynomial of order i
  - N : Maximum degree of Legendre polynomial of order ϱ_i
  - Y_ℓ^m : Spherical Harmonic Basis
  - $\ell_{\max}$: Maximum degree of Y_ℓ^m

- System of Equation

$$\mathbf{A}X_r = \mathbf{F}$$

where

- $k(:= N\left(\ell^2 + m + 1\right) + i \in \{1, 2, \ldots, N\left(\ell_{\max} + 1\right)^2\}), k'$ entry

$$\begin{aligned}[\mathbf{A}]_{k,k'} &= \int_{\mathcal{D}} \tilde{\varepsilon}(\mathbf{x}) \nabla\left(\varrho_i Y_\ell^m\right) \cdot \nabla\left(\varrho_j Y_{\ell'}^{m'}\right) \\ &+ \int_{\mathcal{D}} \tilde{\lambda}(\mathbf{x}) \tilde{\mathcal{F}}\left(\overline{\tilde{w}}(\mathbf{x})\right) \varrho_i Y_\ell^m \varrho_j Y_{\ell'}^{m'} \\ &+ \frac{\ell}{\delta} \int_{\partial B_\delta(\mathbf{0})} \varrho_i Y_\ell^m \varrho_j Y_{\ell'}^{m'},\end{aligned}$$

- $$[\mathbf{F}]_k = \int_{\mathcal{D}} \tilde{f} \varrho_j Y_{\ell'}^{m'} \quad \forall\ k \in \{1, \ldots, N(\ell_{\max} + 1)^2\}.$$

- HSP equation in unit ball [1]

$$\begin{aligned} -\Delta u_e + \kappa^2 u_e^2 &= 0 \quad \text{in } B_1(\mathbf{0}), \\ u_e &= \phi_e \quad \text{on } \mathbb{S}^2 \end{aligned}$$

- u_e can be numerically approximated by $\tilde{u}_e$

$$\tilde{u}_e(r,\theta,\varphi) = \sum_{\ell=0}^{\ell_{\max}} \sum_{m=-\ell}^{\ell} \left[\tilde{\phi}_e\right]_\ell^m \frac{i_\ell(r)}{i_\ell(1)} Y_\ell^m(\theta,\varphi)$$

for $0 \leq r \leq 1,\ 0 \leq \theta \leq \pi,\ 0 \leq \varphi < 2\pi$

[1] Quan, Stamm, Maday: SISC, 41(2), B320-B350, 2019

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  - $\left[\tilde{\phi}_e\right]_\ell^m$: Numerical approximation of $[\phi_e]_\ell^m$ [2]

$$\left[\tilde{\phi}_e\right]_\ell^m = \sum_{n=1}^{N_{\text{leb}}} \omega_n^{\text{leb}} \phi_e(s_n) Y_\ell^m(s_n)$$

[1] Quan, Stamm, Maday: SISC, 41(2), B320-B350, 2019

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- Numerical Integration[1,2]

[1] Haxton: J.Phy.B, 40, 4443, 2007

[2] Parter: JSC, 14, 347-355, 1999

- Numerical Integration[1,2]

$$\int_{\mathcal{D}} h(\mathbf{x}) d\mathbf{x} = \int_{\delta}^{1} r^2 \int_{\mathbb{S}^2} h(r, \mathbf{s}) d\mathbf{s} dr$$

$$\approx \frac{1-\delta}{2} \sum_{m=1}^{N_{\mathrm{lgl}}} \sum_{n=1}^{N_{\mathrm{leb}}} \omega_m^{\mathrm{lgl}} \omega_n^{\mathrm{leb}} \left(\frac{1-\delta}{2}(x_m + 1) + \delta \right)^2$$

$$\times h\left(\frac{1-\delta}{2}(x_m + 1) + \delta, \mathbf{s}_n \right).$$

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- Energy Computation[1]

$$E_s = \frac{\beta}{2}\int_\Omega \rho^{\mathrm{sol}}(\mathbf{x})\psi_r(\mathbf{x}) + \frac{\beta^2\kappa^2\varepsilon_s}{8\pi}\int_\Omega \lambda(\mathbf{x})\left(\psi_r(\mathbf{x})\sinh\left(\psi_r(\mathbf{x})\right) - 2\cosh\left(\psi_r(\mathbf{x})\right)\right)$$

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- Stopping Criteria
  - Global Iterative Process

$$|{E_s}^k - {E_s}^{k-1}|/|{E_s}^k| \leq \mathrm{tol}$$

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$$\frac{\|X_r{}^k - X_r{}^{k-1}\|_{\ell^2}}{\|X_r{}^k\|_{\ell^2}} \le 10 \times \text{tol}$$

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  - Matrix loop

$$\frac{\|{X_{r,i}}^k - {X_{r,i}}^{k-1}\|_{\ell^2}}{\|{X_{r,i}}^k\|_{\ell^2}} \leq 100 \times \text{tol}$$

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  - ε_s: 78.54
  - κ: 0.104 $Å^{-1}$
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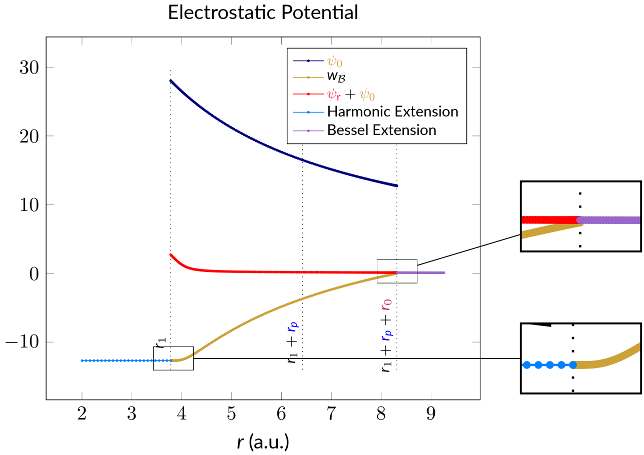
  - Conversion to atomic units

Potential for One Sphere

- Discretisation Parameters: $N = 20$, $N_{\text{lgl}} = 200$
- Geometric Parameters: $r_1 = 2$ Å, $r_0 = 1$ Å, $a = 0$ Å



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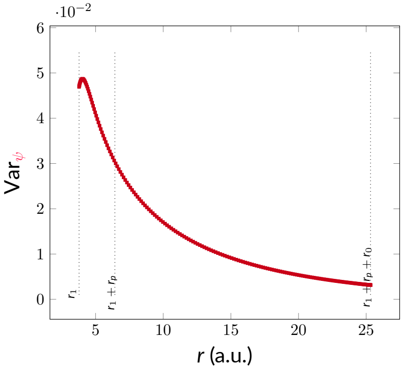
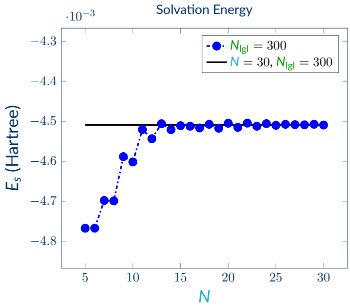
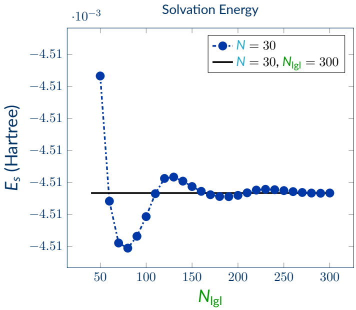


- $\text{Var}_\psi(r) := |\psi_{\text{PB}}(r) - \psi_{\text{LPB}}(r)|$

Effect of Discretisation Parameters

- Discretisation Parameters: $N = 30$, $N_{\text{lgl}} = 300$
- Geometric Parameters: $r_1 = 2$ Å, $r_0 = 5$ Å, $a = 0$ Å





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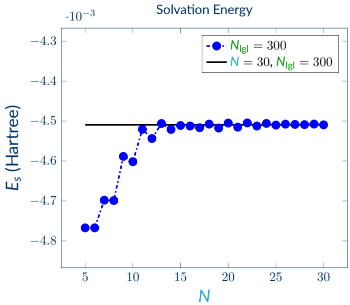
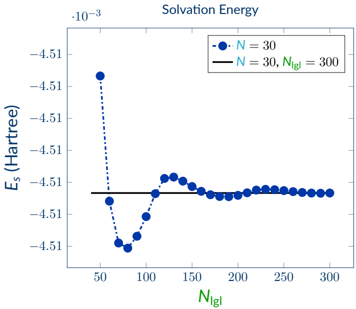
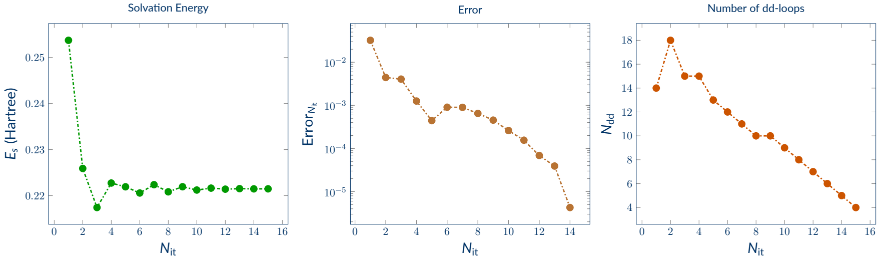




- Similar observations for spherical discretisation

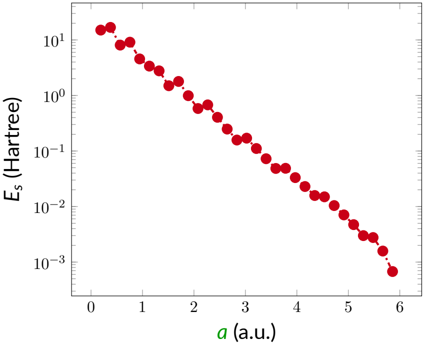
Convergence of Global Strategy

- Caffeine Molecule
- Discretisation Parameters: $N = 15$, $N_{\text{lgl}} = 50$, $\ell_{\text{max}} = 9$, $N_{\text{leb}} = 350$
- Geometric Parameters: $r_0 = 5$ Å, $a = 1$ Å

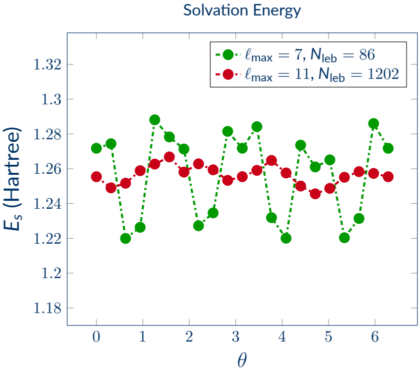


- $\text{Error}_{N_{\text{it}}} := \left| E_s^{\infty} - E_s^{N_{\text{it}}} \right|$

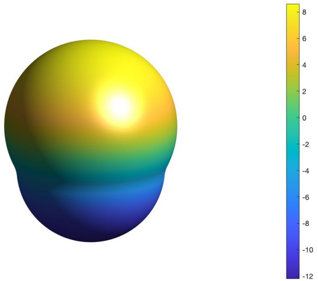
- Hydrogen Fluoride Molecule
- Discretisation Parameters: $N = 15$, $N_{\text{lgl}} = 50$, $\ell_{\text{max}} = 8$, $N_{\text{leb}} = 1202$
- Geometric Parameters: $r_0 = 2$ Å

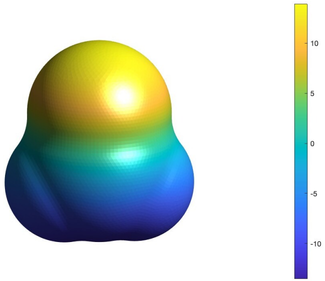


- Hydrogen Fluoride Molecule
- Discretisation Parameters: $N = 15$, $N_{\text{lgl}} = 50$
- Geometric Parameters: $r_0 = 2$ Å, $a = 1$ Å

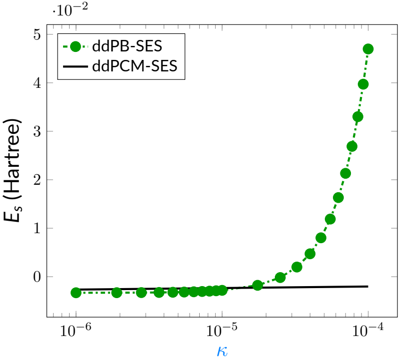


- Visualisation of ψ_{r}
- Discretisation Parameters: $N = 15$, $N_{\mathrm{lgl}} = 50$, $\ell_{\mathrm{max}} = 11$, $N_{\mathrm{leb}} = 1202$
- Geometric Parameters: $r_0 = 1$ Å, $a = 0.5$ Å





- Hydrogen Fluoride Molecule
- Variation of κ
- Discretisation Parameters: $N = 15$, $N_{\mathrm{lgl}} = 30$, $\ell_{\mathrm{max}} = 7$, $N_{\mathrm{leb}} = 86$
- Geometric Parameters: $r_0 = 0$ Å, $a = 0$ Å



- Conclusions[1]
  - Formulation of domain decomposition method for PB equations

[1] J., Stamm, arXiv: 2309.06862, 2023
[2] Nottoli, Herbst, J., Lipparini, Mikhalev, Stamm, ddX: https://github.com/ddsolvation/ddX

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Conclusions and Outlook

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Thank You!

[1] J., Stamm, arXiv: 2309.06862, 2023

[2] Nottoli, Herbst, J., Lipparini, Mikhalev, Stamm, ddX: https://github.com/ddsolvation/ddX